MACHINE LEARNING-BASED PROBABILISTIC STOPPING RULE FOR THE GRASP METAHEURISTIC

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PARADA PROBABILÍSTICA BASEADA EM APRENDIZADO DE MÁQUINA PARA A METAHEURÍSTICA GRASP

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Dezembro/2021

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Metaheurísticas, como Simulated Annealing, Ant Colony, Algoritmos Genéticos e GRASP, são métodos genéricos que são normalmente aplicados a problemas computacionalmente difíceis. Porém, elas normalmente carecem de um critério de parada efetivo, recorrendo a opções genéricas que resultam em desperdício de recursos computacionais e de tempo. A fim de mitigar esse problema, existe para a metaheurística GRASP um critério de parada probabilístico que utiliza a função de distribuição acumulada (FDA) para calcular, a partir de uma dada iteração, a probabilidade de melhorar a solução em iterações futuras. No entanto, apesar de efetivo, ele possui suas próprias deficiências. Especificamente, o cálculo da FDA é relativamente lento e as probabilidades estimadas, em muitos casos, podem divergir significativamente da probabilidade observada em execuções suficientemente longas. Neste trabalho, propõe-se uma alternativa ao critério de parada probabilística baseada em aprendizado de máquina. Esta dissertação mostra que, ao substituir a FDA por modelos baseados em árvore, é possível reduzir o tempo necessário para estimar probabilidades e diminuir a divergência com a probabilidade observada em execuções do GRASP. Também é mostrado que é possível, para um modelo treinado sobre execuções de uma instância de um problema, generalizar para instâncias do mesmo ou de outros problemas, mas com limitações.

Abstract of Dissertation presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Master of Science (M.Sc.)

MACHINE LEARNING-BASED PROBABILISTIC STOPPING RULE FOR THE GRASP METAHEURISTIC

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December/2021

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Metaheuristics, like Simulated Annealing, Ant Colony, Genetic Algorithms and GRASP, are generic methods that are applied to solve problems that are computationally hard. However, they usually lack an effective stopping criterion, relying on generic options that usually result in a waste of computational resources and time. Seeking to mitigate that problem, there is a probabilistic stopping criterion for GRASP that uses the cumulative distribution function (CDF) to calculate, for a given iteration, the probability of improving the current solution in future iterations. Yet, that criterion also has its own drawbacks. Specifically, the CDF can be relatively slow to calculate and the probabilities it estimates, in many cases, can significantly diverge from the probabilities observed in sufficiently large executions. In this work, a machine learning-based alternative to the probabilistic stopping rule is proposed. This dissertation shows that, by replacing the CDF with a tree-based machine learning model, it is possible to reduce the time taken to estimate a probability and reduce the divergence between that probability and the probability observed in sufficiently large executions. It is also shown that it is possible for a model trained on a given instance, of a given problem, to generalize to other instances, even from other problems, but with limitations.

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Chapter 1

Introduction

In this chapter, the problem that motivates this work is presented, as well as a brief description of the contributions effectively achieved and of the text structure.

1.1 Motivation

Metaheuristics, like Simulated Annealing, Genetic Algorithms, Ant Colony, Tabu Search and GRASP are generally employed to problems that are computationally hard, that do not have known optimal solution, where they perform a set of generic procedures in order to achieve sufficiently good solutions. However, despite their success in producing solutions to those problems, they usually lack an effective stopping criterion and decide on whether they should stop searching for an improved solution based on criteria like a total number of iterations, the total execution time, a number of iterations without improvement to the best solution and other options that commonly lead to an unnecessary waste in time and in computational resources.

That waste usually happens because of two different situations. The first is known as *early stopping* and occurs when the execution stops a few iterations away from an improved solution. Having no way to know that a better solution is nearby, the metaheuristic throws away all the computational resources that it spends from the moment it finds the current best solution up until the moment it stops the execution, despite the fact that it could have improved the solution had it continued the execution for a few more iterations.

The second situation, on the other hand, happens when the optimal solution, or a very good local minimum, is found. In those cases, the metaheuristic continues to search for a better solution without knowing that there is very little or no chance for one to be found and, consequently, wastes time and computational resources once again.

In the context of the GRASP metaheuristic [2], those problems are also present and, in order to mitigate them, RIBEIRO *et al.* [1] proposed a probabilistic stopping rule for that metaheuristic. In their work, they showed that the solutions of a GRASP execution follow a normal distribution and used that fact to develop a method that estimates the probability of finding an improved solution in a future iteration, based on the calculation of the cumulative distribution function of the solutions.

However, despite being an effective criterion and also providing a way to define the quality of the of the solution desired, that approach also has its own drawbacks. Specifically, it tends to be relatively slow to calculate the estimates and the probabilities it produces might deviate significantly from the probabilities observed within a sufficiently large execution.

Seeking to mitigate that, in this work, an alternative to the stopping criterion of RIBEIRO *et al.* [1] is proposed, where machine learning is applied to replace the role of the cumulative distribution function. It is shown that that approach can be relatively faster than the original criterion and that it can also generalize across instances of the problem that produced the instance utilized in model training. Generalization across problems is also observed, but with limitations.

1.2 Contributions

The main contribution brought by this work consists in a new probabilistic stopping rule for the GRASP metaheuristic that improves the original stopping rule of RIBEIRO *et al.* [1] through the use of machine learning, being faster to estimate probabilities and, in many cases, capable of obtaining a smaller error when that probability is compared to the expected value within a sufficiently large execution. It also demonstrates that the new approach has generalization capabilities, showing that models trained on an instance from the Set k-Covering Problem can be effectively employed for a stopping criterion for an instance from the Quadratic Assignment Problem and vice-versa, but with some imitations.

1.3 Text Outline

This text is organized in five chapters. In Chapter 2, the background for the work conducted is presented, covering the topics GRASP, probabilistic stopping rule for GRASP, Set k-Covering Problem, Quadratic Assignment Problem and a few tree-based machine learning techniques, called Decision Tree Regression, Random Forest Regression and Extreme Gradient Boosting.

In Chapter 3, the methodology is covered, specifying how the proposed stopping criterion is supposed to work and topics like dataset generation, feature selection, normalization and parameter selection. For this last item, it is done for each of the three machine learning models used in this work.

Finally, in Chapter 4, the results are presented and a brief discussion on model selection is provided, while, in Chapter 5, the conclusion remarks are made and a list of possible future works is provided.

Chapter 2

Background

In this chapter, the techniques and theoretical concepts that support this work are presented. It starts by introducing the GRASP metaheuristic and its probabilistic stopping criterion. Next, it presents a set of tree-based machine learning techniques that are used in this text. Lastly, two optimization problems — the Set k-Covering Problem and Quadratic Assignment Problem — are described.

2.1 A Decision Model for GRASP Metaheuristic

2.1.1 GRASP

GRASP [2] is a multi-start metaheuristic, whose name is an acronym for *Greedy Randomized Adaptive Search Procedures*. In its standard form, it is based in two steps, a construction phase and a local search, that are executed in sequence at every iteration, as shown by Algorithm 1.

In the construction phase, the algorithm builds an initial feasible solution through a greedy randomized search. That search procedure is similar to the usual greedy search. The difference resides in the way that the node expansion occurs. In a greedy search the edge followed is the one that returns the smallest cost (in a minimization problem). Meanwhile, in a greedy randomized search, a *Restricted Candidate List* (RCL) is built, containing the n best edges, and one of them is selected at random and followed.

After the greedy randomized search finishes and an initial solution is obtained, the next step is the execution of a local search, that will investigate the vicinity of that solution, looking for a local minimum. Once it ends, the last step is to update the best solution. That will only happen if the solution produced by the local search has a smaller cost than the current best. Those steps are repeated until a certain stopping criterion, like a total number of iterations, is reached.

In its basic form, a GRASP implementation requires the definition of only one

Algorithm 1: Pseudocode for a simple GRASP implementation.

```
procedure grasp (maxIterations, rclSize)
    bestSolution ← null
    bestCost ← +∞
    for i ← 1 to maxIterations do
        solution ← greedyRandomizedSearch(rclSize)
        solution ← localSearch(solution)
        cost ← getCost(solution)
        if cost < bestCost then
            bestCost ← cost
            bestSolution ← solution
        end
    end
    return bestSolution, bestCost
end
```

or two parameters. The n, that can be an integer or a percentage and represents the RCL size, and the stopping criterion, that can be, among other things, a fixed number of iterations, a number of iterations without improvement to the best solution, etc.

2.1.2 Probabilistic Stopping Rule

The probabilistic stopping rule for GRASP is a method that was proposed by RIBEIRO *et al.* [1]. Based on the fact — demonstrated by the same paper — that the costs of the solutions obtained along GRASP iterations follow a normal distribution, it uses the cumulative distribution function (CDF) of those costs to estimate, for a given iteration, the probability of finding, in the next iteration, a minimum that is, at least, as good as the current best solution. That probability is then compared to a threshold and the execution is stopped if it is surpassed.

In order to better describe it, consider the existence of a random variable X, associated with the objective function value of the local minimum obtained at each GRASP iteration. $f_X(.)$ is its probability distribution function, and $F_X(.)$ its cumulative distribution function. Let $f_1, ..., f_k$ be the set of solutions obtained in the first k iterations, while $f_X^k(.)$ and $F_X^k(.)$ are, respectively, the estimates of $f_X(.)$ and $F_X(.)$, also in the first k iteration. The probability of finding, at iteration $k+1$, a minimum at least as good as the one found up to iteration k (defined as UB^k) is estimated by Equation (2.1).

$$F_X^k(UB^k) = \int_{-inf}^{UB^k} f_X^k(\tau)\, d\tau \tag{2.1}$$

Additionally, if the boundaries of the instance being optimized are available, or trivial ones can be calculated, it is possible to improve the probabilities estimated by truncating the normal distribution. The truncation can happen in only one side, if only one of the bounds is available, or in both sides, if both can be obtained.

After the probability is obtained, the next step is to compare it to a threshold β, that is a value between zero and one that is provided by the user. If, at a given iteration, the estimated probability is less than or equal β, the execution stops, otherwise it continues. If the threshold is never reached, the execution continues indefinitely or until it reaches a secondary stopping criterion (like a maximum number of iterations), that is used to assure that the search will stop at some point. That threshold also doubles as a way to define the quality of the solution to be returned, because the lower the probability, the better the solution obtained is expected to be.

2.2 Machine Learning Based Decision Models

2.2.1 Decision Tree Regression

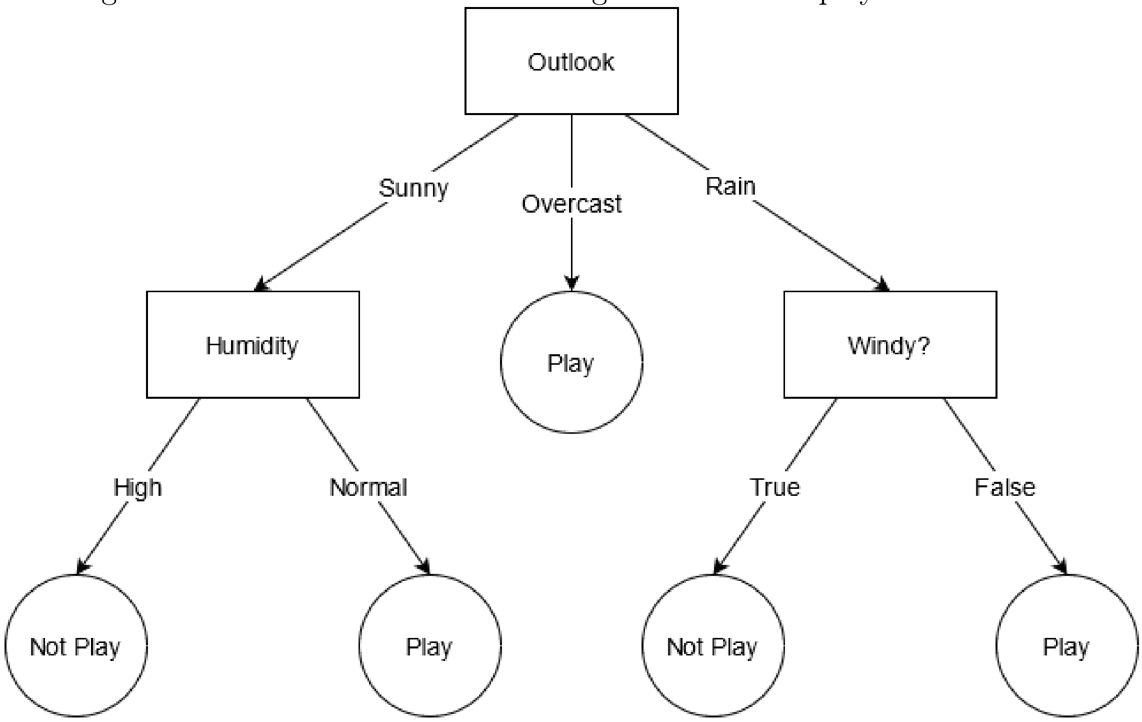
Decision Tree is a simple, yet powerful, machine learning technique. It is a non-linear estimator, that consists in a binary tree that represents a set of rules that are learned from the training data during the training procedure. A decision tree is more often associated to classification tasks, that are those where the predicted variable is categorical. An example of a classification tree, borrowed from QUINLAN [3], can be seen in Figure 2.1.

In that example, the decision that it represents is whether a person should play tennis or not in a given day. In other words, given the set of weather-related input values, that are presented in Table 2.1, it tries to classify them as "play" or "not play".

From that tree, it is also possible to highlight the three main components of a decision tree: the internal nodes, the edges and the terminal nodes. The internal nodes (rectangles) represent, each, an input variable, and each variable might be represented by zero or more nodes within the tree. The first internal node, that sits at the top of the tree, receives an special name, being called the "root". Terminal nodes (circles), on the other hand, represent the output variable and hold one of the possible output values. They are also known as "leaf" nodes. Finally, the edges are what connect all those nodes, and represent the possible values that an input variable is expected to hold. They are called "branches".

To illustrate how such a tree works, imagine an input where $Outlook = Sunny$, $Humidity = Normal$ and $Windy? = True$. In that case, the tree would start by

Figure 2.1: A decision tree for deciding on whether to play tennis or not.



Variable	Values
Outlook	Sunny Overcast Rain
Humidity	High Normal
Windy?	True False

Table 2.1: Input variables and their possible values.

evaluating the value of the variable *Outlook* and, due to its value (*Sunny*), it would evaluate *Humidity* next. The final outcome would then be *Play*, because Humidity has *Normal* as its value. In the end, *Windy*? would not be evaluated.

To achieve a classification tree like the one present in Figure 2.1, multiple approaches are available in the literature, like the ID3 [3] and its extension C4.5 [4]. However, in this text, decision tree is applied to a different kind of problem. Instead of predicting a class, what is needed is a technique that estimates a real value. For that reason, decision tree regression was used.

The use of tree structures for regression problems is not new [5] and dates back the early 60's, when the Automatic Interaction Detection [6], or AID, was proposed. In this work, the algorithm used is the Classification and Regression Trees (CART), that was introduced by BREIMAN *et al.* [7]. As its name already implies, it is more than a simple algorithm to produce regression trees, it integrates procedures to build trees for classification and regression problems.

In order to define how the construction of a regression tree works, let D be a dataset of size n, m be the number of features and $j = 1, ..., m$. $X = \{x_1, ..., x_n\}$ is then the array of observations, $Y = \{y_1, ..., y_n\}$ is the array of targets, and each $x_i = \{x_{i1}, ..., x_{ij}\}$ is an observation, and each y_i is a target (a real number) associated to x_i, where $i = 1, ..., n$. Starting from that definition, CART's procedures can be split in two phases: one to build a maximum tree, and other to choose the right size for that tree. In the first phase, the construction of the tree starts from the root node. From that point, for each feature, all values x_{ij} from that feature are sorted in ascending order and, for each pair $(x_{ij}, x_{(i+1)j})$, the average β is calculated.

With that β in hands, the average of the y_i values to the left of that threshold is calculated, as well as the average of the y_i values to the right of it, resulting in $\beta_<$ and $\beta_>$, as shown in Equations (2.2) and (2.3), respectively, where $I_< = \{i|x_{ij} < \beta\}$ and $I_> = \{i|x_{ij} > \beta\}$.

$$\beta_< = \frac{\sum_{i \in I_<} y_i}{|I_<|} \tag{2.2}$$

$$\beta_> = \frac{\sum_{i \in I_>} y_i}{|I_>|} \tag{2.3}$$

Once all β values and their respective $\beta_<$ and $\beta_>$ are obtained, the next step is to calculate the sum of the squared residuals (SSR) — or the sum of the squared losses — of that threshold, as described by Equation (2.4). The threshold that is chosen to split the data at the root node is the one that produces the smallest SSR, meaning that the data, at that node, will be split by the feature associated to that threshold and based on values smaller than that threshold (to the left) and greater (to the right).

$$SSR = \sum_{i \in I_<} (y_i - \beta_<)^2 + \sum_{i \in I_>} (y_i - \beta_>)^2 \tag{2.4}$$

After the root node is done, that process continues to be executed in a recursive manner. That node will originate two other nodes, those nodes two more each, and so on. However, for each child node, even though β, $\beta_<$, $\beta_>$ and SSR are calculated exactly in the same way, the feature values used for that are the ones "inherited" from its parent. In other words, once a given feature was used to split a given node, for that feature, that node's children will only receive the x_{ij} with respect to the $I_<$ or to the $I_>$ of that parent.

In its standard form, the generation of splits — and child nodes — will only be terminated when a maximum tree is reached. That tree is the one where all leaf nodes have exactly one observation, being impossible to produce further splits. In this case, the output value from that node will be the $\beta_<$ or the $\beta_>$ of its parent, depending on whether it is the left or the right child, respectively.

At this point, the maximum tree should be already able to achieve a low error if evaluated on its training data. However, there will be a good chance that it will have a poor performance on unseen data, because a maximum tree is likely to overfit its training data.

To avoid that, a series o procedures can be used. One of them is to only allow for a split if a node has more than a given number of observations to work with. Another one is to limit the growth of a tree up to a certain depth that, once reached by a given node, no further splits are executed from that node and it becomes a leaf. A third one is to prune the tree, a procedure that varies depending on the type of the tree (regression or classification), but it will not be described in this section because it was not employed in this work.

2.2.2 Random Forest Regression

Decision Trees, as described in Section 2.2.1, are models that are prone to overfitting. However, that only covers part of the problem. While deep trees (specially maximum trees) are prone to overfitting — which generally means a high variance when evaluated on unseen data —, shallow trees are prone to have a high bias, having trouble to correctly estimate even the training data. The strategies briefly mentioned in that same section, like restricting the tree growth up to a certain depth, can help, but it can be hard to find the best parameters (like the maximum depth), that provide the best trade off between bias and variance.

In order to deal with the problem of high variance, one alternative is the use of **b**ootstrapping **agg**regat**ing**, or *bagging*. In that technique, given the existence of a probability distribution P and a dataset D composed of a sample of observations drawn from P, D is used to *learn* P through the use of resampling. Specifically, instead of a single dataset D of size n, several datasets D' of size n' are generated with observations drawn uniformly from D with replacement (those datasets D' are called bootstraps, while the process of producing them is called bootstrapping). After that, each D' is used to train a different model, producing an *ensemble* of models. Once such an ensemble is built, it produces an estimate by simply evaluating its input on every model and then averaging the values returned, if the models are regressors. If they are classifiers, the output from the models can be considered as votes and the ensemble will output the class that received the most votes.

Given the fact that the D' are built by observations sampled with replacement, it is expected that any D' will contain an increasing number repeated values, the larger

n' is. If $n = n'$ and n is a sufficiently large number, the repetitions are expected to account for approximately $1/3$ of the observations in D'.

In the context of decision trees, random forest [8] is a technique that uses bagging to produce an ensemble of decision trees. It differs from a simple bagging — and has *random* in its name — because of the way it trains the models. In its standard definition, the models D' are grown until they reach a maximum tree. However, in order to produce different trees every time, only a randomly selected subset of features is considered for each split.

2.2.3 Extreme Gradient Boosting

The Extreme Gradient Boosting [9], or XGBoost, is an ensemble of trees, capable of Classification and Regression, that uses *boosting* to train its estimators. In boosting, in opposition to bagging, the trees generated are considered weak learners, because they are trained to shallow depths, instead of going up to maximum depth, and have poor performance individually. The idea behind that method is that, by combining a set of weak learners, the ensemble might be able to produce a strong learner. The specific way it works varies from technique to technique.

In Gradient Boosting [10], like in other boosting techniques, a set of weak learners is combined to produce a strong learner. To achieve that, the method consists in an iterative process where, at each step, a new weak model is inserted in the set in order to improve the predictions produced by the ensemble.

Firstly, given a dataset $D = \{(x_i, y_i)\}_{i=1}^{n}$, where n is the number of observations it contains, and a differentiable loss function $L(y, F(x))$, where F is the function that represents the entire ensemble, the algorithm starts by producing a constant function $F_0(x)$, that can be seen as the first model in the ensemble. That value is calculated through Equation (2.5).

$$F_0(x) = \underset{\gamma}{\operatorname{argmin}} \sum_{i=1}^{n} L(y_i, \gamma) \tag{2.5}$$

After that first model is obtained, a loop is executed for M iterations. In each iteration $m = 1, ..., M$, the first task is to calculate the pseudo-residuals g_{im} through the gradient presented in Equation (2.6). With those residuals in hand, the algorithm then proceeds to fit a weak learner to them, instead of the usual y_i's. In other words, the new model $F_m(x)$ is trained on the dataset $D_m = \{(x_i, g_{im})\}_{i=1}^{n}$. That is done in order to compensate for the error of the previous models and, consequently, reduce the error of the ensemble.

$$g_{im} = -\left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, ..., n \tag{2.6}$$

Once the model is trained, the next step to be executed within the same iteration is to determine the terminal regions of the model. For regression trees, this step consists in labeling each leaf of the tree as a terminal region R_{jm}, where each $j = 1, ..., J_m$ is a number associated with a single leaf and J_m is the total number of leaves in the tree produced at iteration m.

After the definition of the terminal regions, there are two remaining steps to be done in an iteration. The first is to calculate the output values of each leaf j. That is done through Equation (2.7).

$$\gamma_{jm} = \underset{\gamma}{\operatorname{argmin}} \sum_{x_i \in R_{jm}} L(y_i, F_{m-1}(x_i) + \gamma) \tag{2.7}$$

The second remaining step consists of updating $F_m(x)$, which is done by Equation (2.8), and producing the predictions of the ensemble at iteration m. In that equation, the variable ν represents the learning rate (also known as the regularization parameter), that is a value between 0 and 1. It is a penalty applied to the predictions of the models that aims to reduce the chances of over fitting. After iteration M finishes, the last step is to output $F_M(x)$, that is the model that constitutes the entire ensemble.

$$F_m(x) = F_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} 1 R_{jm}(x),\ 0 < \nu \leqslant 1 \tag{2.8}$$

When compared to Gradient Boosting, XGBoost works in a similar manner, but with major differences. Two of them are the trees it uses, that can be built in multiple ways, differing from standard CART trees, and the fact that regularization is not limited to the learning rate, being also present in tree construction. Further details about these two aspects can be found in the original work.

In the XGBoost algorithm (covered here in a generic way, based on NIELSEN [11], for simplicity), like in the standard gradient boosting, the first step is to create the constant function $F_0(x)$, that is calculated in the same way. After that, in each iteration m, not only the gradients are calculated, but also the hessians (second order derivatives), according to Equations (2.9) and (2.10), respectively.

$$g_{im}(x_i) = \left[\frac{\partial L(y_i, F(x_i))}{\partial F(x_i)}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, ..., n \tag{2.9}$$

$$h_{im}(x_i) = \left[\frac{\partial^2 L(y_i, F(x_i))}{\partial F(x_i)^2}\right]_{F(x)=F_{m-1}(x)} \quad \text{for } i = 1, ..., n \tag{2.10}$$

After that, the tree associated with iteration m is trained on the dataset $D_m = \{(x_i, -\frac{g_{im}(x_i)}{h_{im}(x_i)})\}_{i=1}^{n}$ and the output is given by Equation (2.11), where ϕ represents a base learner (in this case, the tree). Once it is done, the model is updated by

Equation (2.12).

$$\hat{\phi}_m(x) = \underset{\phi}{\mathrm{argmin}} \sum_{i=1}^{n} \frac{1}{2} h_{im}(x_i) \left[-\frac{g_{im}(x_i)}{h_{im}(x_i)} - \phi(x_i) \right]^2 \tag{2.11}$$

$$F_m(x) = F_{m-1}(x) + \nu \hat{\phi}_m(x) \tag{2.12}$$

After iteration M is executed, like in the standard gradient boosting, the last step performed by the algorithm is to return the model $F_M(x)$, that constitutes the ensemble.

Lastly, it is important to mention that XGBoost is a highly customizable technique and, for that reason, it is not possible to cover every single aspect of it in this text. However, in Chapter 3, the parameters used in the models trained in this work are presented. In that moment, where needed, further reference will be provided (but not described).

2.3 Test Optimization Problems

In order to develop and test the technique proposed by this text, two optimization problems that were used by RIBEIRO *et al.* [1] were employed in this work. They are the Set Covering Problem (specifically, a variant called "Set k-Covering Problem") and the Quadratic Assignment Problem. They are described in the sections 2.3.1 and 2.3.2, respectively.

2.3.1 Set k-Covering

The Set Covering Problem (SCP) is an optimization problem that is known to be NP-Hard [12]. In its standard definition, there is a set $I = \{1, ..., m\}$ and a set $P = \{P_1, ..., P_n\}$, where each P_j, with $j = 1, ..., n$, is a subset of I (it *covers* a subset of elements of I) and is associated with a cost c_j. The aim of the optimization is to find a set J that is the union of a number of subsets P_j of P such that $J = I$ and the sum of the associated costs c_j is minimal.

In order to provide a simple example, consider a set $I = \{1, 2, 3, 4, 5\}$ and a set $P = \{\{1, 2, 5\}, \{1, 2, 4\}, \{1, 3\}, \{4, 5\}, \{2, 3\}, \{2\}\}$ of subsets of I, with each c_j equal to the number of elements in its respective P_j or, in other words, $c_1 = 3$, $c_2 = 3$, $c_3 = 2$, $c_4 = 2$, $c_5 = 2$, $c_6 = 1$. The union of subsets of P_j that would produce the smallest total cost is $J = \{P_3, P_4, P_6\}$, with a total cost of 5.

The Set k-Covering Problem [13] is a variation of the traditional SCP, with the additional restriction where each element of I must be covered at least k times. In this case, if considered the example that was just provided, the optimal solution would then become $J = \{P_1, P_2, P_3, P_4, P_5\}$ for $k = 2$, with a total cost of 12.

In this work, the abbreviation SCP will always mean the Set k-Covering Problem, because the traditional Set Covering Problem was not employed in any of its stages. Additionaly, it should always be assumed that $k = 2$. The GRASP implementation for SCP that was used in this work is the same employed by RIBEIRO *et al.* [1] in their work and comes from PESSOA *et al.* [14].

2.3.2 Quadratic Assignment

The Quadratic Assignment Problem (QAP) is a classic problem in the fields of optimization and operations research that was first introduce by KOOPMANS and BECKMANN [15] and was shown to be NP-Hard by SAHNI and GONZALEZ [16]. In its definition, there is a set of n facilities and a set of n locations. For each pair of facilities, there is an associated flow and, for each pair of locations, there is an associated distance. The goal of the optimization problem is to allocate facilities to locations such that the sum of the product between the distances and the flows is minimal.

Formally, given a set of facilities $F = \{f_1, ..., f_n\}$ and a set of locations $L = \{l_1, ..., l_n\}$, there is a matrix of flows $A^{n \times n} = (a_{i,j})$, where each $a_{i,j} \in \mathbb{R}^+$ is the flow between facilities f_i and f_j, and a matrix of distances $B^{n \times n} = (b_{i,j})$, where each $b_{i,j} \in \mathbb{R}^+$ is the distance between locations l_i and l_j. With those matrices as input, the QAP considers an assignment $p : \{1, ..., n\} \rightarrow \{1, ..., n\}$ with cost $c(p)$ defined by Equation (2.13) and searches for a permutation vector $p \in \Pi_\text{n}$ that minimizes $c(p)$, where Π_n is the set of all permutations of $\{1, ..., n\}$.

$$c(p) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j} b_{p(i),p(j)} \tag{2.13}$$

The GRASP implementation for QAP that was used in this work is the same used by RIBEIRO *et al.* [1] and comes from OLIVEIRA *et al.* [17].

Chapter 3

AIISR: AI Inspired Stopping Rule For GRASP Metaheuristic

In this chapter, a machine learning based approach to the probabilistic stopping rule for GRASP is described. It starts by providing a general overview of the method, that was called *AI Inspired Stopping Rule For GRASP Metaheuristic* (just a catchy name). After that, the remaining sections cover the datasets used in this work, feature selection and parameter selection for the machine learning techniques that were employed.

3.1 Overview

The probabilistic stopping rule of RIBEIRO *et al.* [1], described in Section 2.2, is an effective stopping criterion for GRASP that alleviates the problem of early stopping, where the search for a solution stops while there is still a relevant chance of finding an improved solution in upcoming iterations, and the problem that arises when the global optimum (or a very good local minimum) is found, but the search continues, because the metaheuristic, in its standard form, has no way to recognize that a solution is indeed optimal. Additionally, it also allows the user to have more control over the quality of the solution, because the probability threshold that it introduces also serves as a measure of quality for the solution sought.

However, despite those benefits, it also has some drawbacks. The most notorious is the time that it takes to calculate the probability of finding a minimum in the next iteration. It happens because that probability is obtained by calculating the Cumulative Distribution Function (CDF) of the distribution of the costs of GRASP iterations, a process that can demand a significant amount of time.

Another problem that is also evident is that the probabilities calculated by the CDF can significantly diverge from sample probabilities observed in sufficiently large executions. In other words, for a given iteration, extracted from a very long execution, the probability of finding a minimum, when calculated on future costs within the execution, can be considerably smaller than one estimated by the CDF (this behavior is shown in Chapter 4).

In order mitigate those limitations, the method proposed by this work replaces the CDF by a machine learning model, that can be any non-linear model that is capable of performing regression tasks, like neural networks, polynomial regression, support vector regression (with non-linear kernels), decision tree regression, among others. In this case, a model is trained on data collected from a series of sufficiently large executions of a given problem instance and, like the CDF, for a given iteration, it is used to estimate the probability of finding a minimum in the next iteration.

Initially, the model produced was expected to work only for the instance it was trained on and, considering that multiple large executions were already performed, the usefulness of such a model would be questionable. Despite that, and considering that GRASP solutions follow a normal distribution, this work evaluates and shows the possibility of applying a model trained on a given instance to estimate the probability of finding new minimums for other instances from the same problem and even for instances of other problems. By doing so, the proposed method manages to achieve some degree of generality, being competitive when compared to the probabilistic stopping rule of RIBEIRO *et al.* [1], that has in its generality one of its main strengths. Details on how that can be done are provided in Section 4.4.

Finally, the remaining element of the probabilistic stopping rule is kept the same as proposed by RIBEIRO *et al.* [1]. The threshold β is a value between 0 and one 1 that is used to stop the search once the probability returned by the machine learning model is equal or smaller than it.

3.2 Datasets

In order to generate a model for a given instance, a dataset composed of a number of sufficiently large executions of that instance is necessary. How many executions and how large they should be are questions that do not have a straight answer and depend on experimentation.

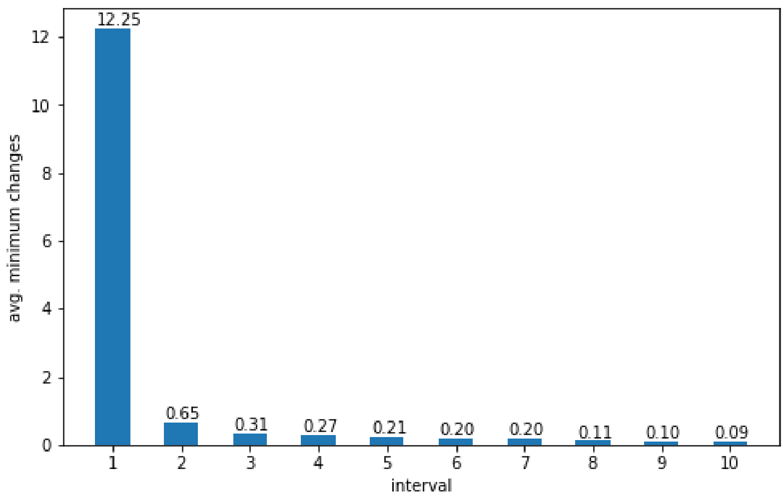
In this work, the number of iterations for each execution was loosely based on the approach taken by RIBEIRO *et al.* [1] to evaluate their own technique. In their paper, they validate the probability p_k, produced by their estimator $F_X^k(.)$ in a given iteration k, where the current minimum is UB^k, by comparing p_k to the number of minimums c_k found in the future. Specifically, they observe the interval $(k, k + 1\,000\,000)$ and count all values smaller than or equal to UB^k within it. To convert p_k to a number of minimums, they simply multiply it by $1\,000\,000$. In the end, that approach results in executions o variable sizes, and always with more than 1 000 000 iterations.

In the present work, on the other hand, seeking to avoid executions of varying sizes, the number of iterations per execution was limited to 1 000 000 and, for a given iteration k, where the current minimum is UB^k, the number of future minimums c_k was obtained from the interval (k,1 000 000) and limited to values strictly smaller than UB^k. To produce a probability from that number, c_k was divided by 1 000 000.

That difference in methodology is justified by a few factors. The first is the difficulty that would be faced if executions of varying sizes were to be employed. It would take longer to produce them and many of the iterations would only serve to calculate the number of future minimums, which could be considered a waste of computational resources and time.

The second reason for that is the fact that most of the changes in minimum usually occur within the first one hundred thousand iterations, making the number of iterations considered when evaluating the number of future minimums greater than 900 000 in most cases (if the execution has 1 000 000 in total). To prove that, Figure 3.1 shows, for the datasets employed in this work for model training (11 in total, from the instances covered in Section 3.2.1), the average number of minimum changes observed within each one hundred thousand iterations of their executions. In that Figure, it is possible to see that, for the first 100 000 iterations, that number is 12.25. On the other hand, for all the other intervals, that average is always inferior to 1.

Figure 3.1: Average number of minimum changes at every 100 000 iterations in executions of the datasets employed for model training. On the x-axis, 1 represents the interval $(1, 100\,000)$, 2 the interval $(100\,000, 200\,000)$, 3 the interval $(200\,000, 300\,000)$, and so on.



The third — and last — reason for that difference in methodology is the fact that the CDF estimates, for a given iteration, the probability of finding a minimum that is, at least, as good as the current one (and not one that is indeed better), because it leads to a situation where those estimates can be seen as overestimates of the real probability of finding a truly improved solution.

In the case of this work, on the other hand, the probabilities utilized in the datasets can be considered underestimations of the reality, because only the number of solutions better than a current minimum are considered as remaining minimums, and also because that number is counted in an interval inferior to one million iterations. However, working with underestimates is not necessarily negative, because it also brings two major advantages. One is that, in early iterations, that number might be closer to reality than the estimates produced by the CDF, because it does not include repetitions of a current minimum. Meanwhile, the other advantage is the fact that the probability will always reach zero within an interval of 1 000 000 iterations, allowing for the stopping rule to operate with thresholds of up to 10^{-6}, something that is not always possible with the method of RIBEIRO *et al.* [1] (instances SCP are an example of that, as they comment in their work).

Now, regarding the number of executions in the datasets, each consisted of 20 different executions (generated with different seeds), totalling 20 000 000 observations per dataset. That number of executions was based on early tests conducted during the development of this work and is related to how many were needed to have a regressor — during that time, a MLP neural network — producing a small error on training and test sets. At that time, tests were conducted on datasets with 5, 10 and 20 executions, that had their data split with 75% of the iterations used for training and 25% used for test.

With regard to training and validation of the models, the procedure used in this work was 10-fold cross-validation, where the final model (trained on all 20 000 000 observations available in a dataset) is the one considered in all tests present in the sections in this chapter and in the tests presented in Chapter 4. Another important information is that, for each fold, the validation set was composed of 2 complete executions ($\frac{20}{10} = 2$) not present in the training set. This was done in order to avoid the leakage of information from the validation executions into the training set built during that fold. The metrics used to produce the cross-validation scores were the mean absolute error (MAE) and the root-mean-square error (RMSE). The reason for two metrics is the fact that they complement each other. While the MAE allows the observation of the average error across the data, the RMSE allows the detection of large deviations.

3.2.1 Selected Instances

In order to develop and demonstrate the method proposed by this work, two optimization problems were employed. They are the Set k-Covering (SCP) and the Quadratic Assigment (QAP), that are described in Sections 2.3.1 and 2.3.2, respectively. The choice for those problems was based on their use by RIBEIRO *et al.* [1] to evaluate their own technique. For the SCP problem, the source for the instances employed in this work was a library of instances of problems of operational research called OR-Libray [18]. From there, the instances applied to this work were the *scp42*, the *scp47*, the *scp55*, the *scpa2* and the *scpb5*. Among them, the first four were also used by RIBEIRO *et al.* [1] in their paper, while the last was randomly picked from the biggest scp*xx* instances available in that source. In Table 3.1, the characteristics of those instances are shown (for further information, check Section 2.3.1).

instance	m	n
scp42	200	1000
scp47	200	1000
scp55	200	2000
scpa2	300	3000
scpb5	300	3000

Table 3.1: Characteristics of the SCP instances.

As for the problem QAP, the instances utilized were the *tai30a*, the *tai35a*, the *tai40a*, the *tai50a*, the *tai100a* and the *tai100b*, that were obtained from a library called QAPLIB [19]. As in SCP instances' case, the first four were also present in RIBEIRO *et al.* [1], while the last two were not and were picked for the same reason *scpb5* was. The characteristics of those instances are available in Table 3.2 and further details in Section 2.3.2.

instance	n
tai30a	30
tai35a	35
tai40a	40
tai50a	50
tai100a	100
tai100b	100

Table 3.2: Characteristics of the QAP instances.

Apart from the instances listed in this section, others were also used in this work and are listed in Tables A.1 and A.2. However, those were not utilized to produce datasets to train models and, for that reason, were not included directly in this section. For each of them, only 10 executions were generated.

3.2.2 Prominent Features

The datasets used in this work consist of data obtained from iterations collected during the execution of a group of instances. Initially, the immediately available features for a given iteration are its sequence number and the cost obtained for the solution produced. However, other features can also be derived from these. In Table 3.3, five other possibilities are listed.

Feature	**Type**	**Description**
iteration	integer	iteration number
cost	float	solution cost
best_cost	float	smallest cost up to the current iteration
best	boolean	flag telling if best_cost changed in the current iteration
iterations_since_last_min	integer	iterations since best_cost last appeared
iterations_since_best_cost	integer	iterations since the best_cost last changed
total_single_mins_found	integer	number of times best_cost changed up to the current iteration

Table 3.3: Features derived from an iteration.

Those prominent features were considered based on two factors: its dependence on cost value and its independence from it. The dependent one is *best_cost*. For a given iteration of a given execution, it aims at tracking the improvement of the solution and, for that reason, it represents the smallest cost found until that iteration. The independent ones, on the other hand, track events that occur during the execution. Specifically, they record *if*, *when* and *how many times* the solution improved. That knowledge is represented by the feature *best*, the combination of features *iterations_since_last_min* and *iterations_since_best_cost*, and the feature *total_single_mins_found*, respectively.

Finally, despite not being a training feature, another variable that must be mentioned is the target variable. In this work, the value that was used as the target is the number of remaining minimums (referred in this text as *remaining_mins*) that are expected to be found in upcoming iterations (within a given execution). It was used, instead of the probability, because it was easier to interpret error metrics in that way (if compared to numbers between zero and one). In the end, to obtain the probability, the user of this methodology could simply divide the number of remaining minimums by 1 000 000 (as mentioned earlier in this chapter).

3.2.3 Normalization

In this work, it is proposed that models trained on executions obtained from a given instance of a given problem can be used to replace the CDF employed by RIBEIRO *et al.* [1] in their probabilistic stopping rule. By doing so, for a given iteration of an unknown instance, those models can estimate the probability of improving a solution in future iterations.

However, at first glance, that approach stumbles on a problem related to the range of cost values produced by GRASP iterations, that can widely differ from instance to instance. If, for an instance A, the lower and upper bounds for cost value are, respectively, 100 and 50000, and, for an instance B, they are, respectively, 8 000 000 and 20 000 000, a model trained on data from instance A is expected to not be able to properly estimate anything for iterations coming from B.

Given that situation, in this work, all datasets were normalized. That step was taken in order to make all the features in those datasets within the same range. Specifically, the MinMaxScaler available in the machine learning library *scikit-learn*[1] (version 0.23.2) was used for that purpose, while the feature range employed was $(0, 1)$. The boundaries used to normalized the features that are independent from cost are available in Table 3.4.

feature	min. value	max. value
iteration	1	1000000
best	0	1
iterations_since_last_min	1	1000000
iterations_since_best_cost	1	1000000
total_single_mins_found	1	100

Table 3.4: Range of the features that are independent from *cost*.

As for *cost* and *best_cost*, the lower and upper bounds for SCP instances are available in Table A.1, while the ones for QAP instances are presented in Table A.2. To obtained those values, different sources were used. The lower bounds for SCP instances come from the linear relaxations that are available in PESSOA *et al.* [14]. For QAP instances, the lower bounds were extracted from the QAPLIB [19]. In that case, in situations where the bound was not available, the cost of the feasible solution was used instead.

The upper bounds, on the other hand, were calculated utilizing different approaches for each problem. For QAP instances, where the instance files are composed by the number of facilities n, the matrix of flows A and the matrix of distances B, the upper bound UB_{QAP} was obtained by Equation (3.1), where a is a vector of

[1]Library scikit-learn: <https://scikit-learn.org/stable/>.

length n^2 containing all the elements of A (sorted in descending order), and b is a vector of length n^2 containing all elements of B (also sorted in descending order).

$$UB_{QAP} = \sum_{i=1}^{n} a_i b_i n \tag{3.1}$$

For the SCP problem, the value is calculated as described in RIBEIRO *et al.* [1]. In this case, each instance file represents a constraint matrix of dimensions $m \times n$, where m and n are as presented in Section 2.3.1. That means that each column represents a set P_j. However, in each file, the content is not the matrix itself, but metadata about it. In its first line, it contains the values of m and n. After that, there is a list of costs c_j for each column. Finally, for each line $l = 1, ..., m$ of the matrix, there is a list of data about it, containing the number (amount) of columns that cover l and a list with the numbers j of those columns.

Given that data, the upper bound was calculated according to Algorithm 2, where k is also as defined in section 2.3.1. As for the other parameters passed to that procedure, *covColumns* is an array of length m where each position represents a value l and holds an array that contains the values j that cover l. *colCost*, as its name already states, is an array of size n where each position contains the cost for a given column j.

Algorithm 2: Pseudocode to calculate the upper bound for SCP instances.

```
procedure calculateUB(k, m, covColumns, colCosts)
    ub ← 0
    for p ← 1 to m do
        lenCovColumns ← length(covColumns[p])
        costs ← array(lenCovColumns)
        if lenCovColumns < k then
            return null
        end
        for q ← 1 to lenCovColumns do
            costs[q] ← colCosts[covColumns[p][q]]
        end
        costs ← sortDescending(costs)
        for r ← 1 to k do
            ub ← ub + costs[r]
        end
    end
    return ub
end
```

3.3 Feature Selection

Considering the features obtained in Section 3.2.3, not all of them are necessarily relevant for estimating the target variable. In order to verify that, the correlation matrix, available in Table 3.5, was calculated using the Pearson Correlation Coefficient, that produces values between -1 and 1. For values above 0.5, it is considered that two variables have a moderate to strong correlation, while a value bellow -0.5 means a negative (inverse) moderate to strong correlation. Values between -0.5 and 0.5 mean a weak correlation, being 0 the only exception, because it means no linear correlation at all.

	(1)	(2)	(3)	(4)	(5)	(6)	(7)	(8)
iteration (1)	1	-0.00	-0.69	-0.00	0.72	0.72	0.74	-0.02
cost (2)	-0.00	1	0.00	-0.00	-0.00	-0.00	-0.00	-0.00
best_cost (3)	-0.69	0.00	1	0.03	-0.38	-0.38	-0.94	0.16
best (4)	-0.00	-0.00	0.03	1	-0.00	-0.00	-0.02	0.24
iterations_since_last_min (5)	0.72	-0.00	-0.38	-0.00	1	0.99	0.36	-0.02
iterations_since_best_cost (6)	0.72	-0.00	-0.38	-0.00	0.99	1	0.36	-0.02
total_single_mins_found (7)	0.74	-0.00	-0.94	-0.02	0.36	0.36	1	-0.10
remaining_mins (8)	-0.02	0.00	0.16	0.24	-0.02	-0.02	-0.10	1

Table 3.5: Average of the correlation between the features and *remaining_mins* across a series of different executions, from different instances and problems.

To obtain that table, two executions were select from each instance listed in Tables 3.1 and 3.2 and, for each execution, the correlation matrix was calculated. After that, those correlation matrices were merged into one single matrix, where the value in each of its positions is the average of the correlation values obtained from each execution for the pair of features that that position represents.

Based on the values present in that table, it is possible to identify that the features with the highest — yet weak — correlation to the target variable *remaining_mins* are *best_cost*, *best* and *total_single_mins_found*, making them the most prominent combination of features to be used to train the models. However, after checking the correlation between those those three features, *best_cost* shows a strong negative correlation with *total_single_mins_found*. Because of that, the most prominent combination appears to be *best_cost* and *best*, because *best_cost* is more correlated to *remaining_mins* than *total_single_mins_found*, leading to the combination (A) shown in Table 3.6.

In that same table, four other combinations are listed. Initially, those aimed to be just simple tests and did not take into account the correlation between the features. Combinations (B), (C), and (D) were considered in order to verify the impact of adding the features *iteration* and *cost*. (E), on the other hand, was contemplated to assess the impact of using features that do not depend directly on cost. However, it does not include *best* because the change of *best_cost* is an event that could be identified through the changes in *iterations_since_best_cost*.

identifier	features
(A)	*best_cost*, *best*
(B)	*iteration*, *cost*, *best_cost*
(C)	*iteration*, *cost*, *best*
(D)	*iteration*, *cost*, *best_cost*, *best*
(E)	*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*

Table 3.6: Combinations of features evaluated in this work.

Finally, it is important to note that the use of the correlation matrix alone for feature selection might not be the best approach, given the fact that there are more powerful alternatives for that same purpose and that decision trees already perform feature selection internally when they are built (the splits it performs are a form of feature selection). However, that method was employed for its simplicity and in order to reduce training time, because the larger the feature set is, the longer the training is expected to take.

3.4 Parameter Selection

In the research conducted, three tree-based machine learning algorithms were used to demonstrate the proposed method. They are Decision Tree Regression, Random Forest Regression and Extreme Gradient Boosting, and were chosen because they are usually fast to train. In the following sections, the process of choosing the parameters for each of them is described.

However, it is important to point out that, in this work, its author did not aim to find optimal parameters for those techniques. Instead, the objective was to find a set of parameters that, for each model, produces an acceptably low cross-validation score and, at the same time, makes it fast to train. That decision was made for two reasons. The first, and more obvious, is the fact that, if the training takes too long, the method proposed by this text might become unappealing. The second reason, on the other hand, is related to the number of models being evaluated. With 3 machine learning techniques, 5 feature combination and 11 datasets, fine tuning all 165 models originated from that is not a practical task. The number of models is also what made the feature set (*best_cost*, *best*) and the dataset for the instances *scp42* and *tai100a* be the only ones considered as reference for parameter selection.

Another relevant information that must be provided is that the Decision Tree Regression and Random Forest Regression implementations used in this work come from the library *scikit-learn*[2] (version 0.23.2). The Extreme Gradient Boosting implementation, on the other hand, is from the library *XGBoost*[3] (version 0.90).

Finally, all the training times reported in the next three sections were obtained by training the models on virtual machines running on Kaggle[4], that were powered by a 4-core virtual CPU, had 16GB of RAM and ran Ubuntu 18.04.5 LTS as its operating system (as of July 2021). The specifics about CPU, RAM and storage were not available, but the processor can be a Xeon, from Intel, or an Epyc, from AMD.

3.4.1 Decision Tree Regression

Decision Tree, as described in Section 2.2.1, is a simple machine learning technique that is very fast to train, but is prone to overfit the training data. In order to avoid that problem, in this work, the approach taken was to limit the tree depth. The reason for that was the fact that, among the available options, it is possibly the fastest. In Table 3.7, it is possible to see that, among the maximum depths tested, bellow depth 10, no relevant improvement in the cross-validation score was observed. For that reason, for all Decision Tree Regression models, the maximum depth that a tree can reach was set to 10. The time required to train those models was also very low, taking less than 30 seconds for each.

max. depth	**training time (s)**	**CV Score (MAE)**	**CV Score (RMSE)**
2	5.11	15.056	316.692
5	12.32	7.129	62.309
10	23.05	1.899	34.014
15	27.96	2.077	34.041
20	34.23	2.077	34.041

max. depth	**training time (s)**	**CV Score (MAE)**	**CV Score (RMSE)**
2	5.59	14.115	329.301
5	13.47	5.340	68.275
10	25.22	1.669	38.463
15	30.57	2.099	38.411
20	30.66	2.162	38.412

Table 3.7: Cross-validation scores observed for decision tree regressors trained on *scp42* (left) and *tai100a* (right) datasets, using the combination of features (*best_-cost*, *best*) and varying maximum depths. Training time refers to the time taken to train the final model of the cross-validation.

It is important to note that, if the scores in Table 3.7 were common errors, there would be a chance that, even at the chosen depth, the tree would be already overfitting the training data, because no improvement was observed by increasing the maximum depth beyond that. However, considering that they are cross-validation scores, that does not seem to be the case, because it shows that all the models created during the cross-validation were able to generalize to their respective validation sets.

[2]Library scikit-learn: <`https://scikit-learn.org/stable/`>.
[3]Library XGBoost: <`https://xgboost.readthedocs.io/en/latest/`>.
[4]Kaggle: <`https://www.kaggle.com/`>.

3.4.2 Random Forest Regression

In a Random Forest, there are three main parameters to be chosen. They are the number of trees that compose the ensemble, the number of observations used to train each tree, and the number of features to be randomly selected as candidates for a split. Other than those, an additional parameter is the stopping criterion for the expansion of the trees, that can be used if the construction of the maximum trees is not desired.

For this work, the number of observations used to train a tree was set to be the size of the entire training set. In practice, according to what is presented in Section 2.2.2, that means that each tree is trained on, approximately, two thirds of the observations present in the training set.

As for the number of candidate features in each split, the value used was the total number of features available. That has a drawback of turning the Random Forest into a simple ensemble of *bagged* trees, but that was done for two reasons. The first is the small number of features available, because only (*best_cost*, *best*) was used for parameter selection. The second, on the other hand, is that that value is recommended by the authors of the library scikit-learn in [20] and [21].

num. trees	**max. depth**	**training time (s)**	**CV Score (MAE)**	**CV Score (RMSE)**
10	5	50.20	6.361	84.120
10	10	94.61	1.953	72.277
30	5	126.67	6.522	84.664
30	10	204.80	1.951	73.126
50	5	173.83	6.539	84.052
50	10	341.11	1.945	72.771

Table 3.8: Cross-validation scores observed for random forest regressors trained on the *scp42* dataset, using the combination of features (*best_cost*, *best*) and varying the number of trees and maximum depth. Training time refers to the time taken to train the final model of the cross-validation.

Lastly, the number of trees in the ensemble and the stopping criterion for tree expansion were chosen. In Table 3.8, it is possible to observe that, for the values tried for those two parameters, there is no relevant advantage for going past 10 trees, making that value the one selected. The maximum depth, on the other hand, was set to 10 based on the observation made in Section 3.4.2 (that there is little to no gain for going past it) and for fears of increasing training time.

3.4.3 Extreme Gradient Boosting

Extreme Gradient Boosting is an ensemble of trees that goes beyond the usual Gradient Boosting and comprises an entire framework that is highly customizable.

In this work, due to the fact that the models used must be fast at training on the datasets available and that, consequently, optimal results are not what is sought, most of the customization options were left unchanged. However, some of them were changed. They are the booster, the maximum depth of the trees and the number of trees that comprise the ensemble.

Starting from the booster, in this work, all XGBoost models employed the booster DART [22]. The reason for that was the fact that, in preliminary tests, it was the option that provided the best results.

The maximum depth and the number of trees were chosen partially based on tests. In Table 3.9, it is possible to see that, regardless of maximum tree depth, as the number of trees grows, the error gets reduced. However, at the same time, the training time increases.

For this work, the values picked for those two parameters were 10 for depth and 20 for number of trees. For the maximum depth, that value was picked because it is already being employed by the other techniques, so, despite not offering any relevant gain if compared to a maximum depth of 5, it ended up being chosen. As for the number of trees, with a maximum depth of 10, going past 20 trees requires a significant training time.

max. depth	**num. trees**	**training time (s)**	**CV Score (MAE)**	**CV Score (RMSE)**
5	10	56.64	6.919	347.266
5	20	113.30	4.268	140.769
5	30	175.75	2.847	66.359
5	50	336.09	1.972	38.226
10	10	104.09	4.587	346.017
10	20	214.95	2.521	139.698
10	30	347.80	2.036	65.813
10	50	715.68	1.985	38.167

Table 3.9: Cross-validation scores observed for XGBoost regressors trained on the *scp42* dataset, using the combination of features (*best_ cost*, *best*) and varying the number of trees and maximum depth. Training time refers to the time taken to train the final model of the cross-validation.

Chapter 4

Experimental Results

In this chapter, a series of experients and their results are presented. It starts by describing the computational environment where the experiments were run and, after that, the results for the evaluation of the models on unknown instances and problems are shown. In the end, a short discussion on model selection is provided.

4.1 Computational Environment

In order to conduct the tests presented in this chapter, the computational environment utilized was the supercomputer *Lobo Carneiro*, from the *Núcleo de Atendimento à Computação de Alto Desempenho*[1] (NACAD), a department at Federal University of Rio de Janeiro. Specifically, the resources used were a single node of that computer, comprising two CPUs Xeon E5-2670v3 (totalling 48 threads) and 64GB of RAM. The operating system was SUSE Linux Enterprise Server 12. Storage specifications were unavailable, however, the *Lobo Carneiro* has a total of 60TB of high-speed network storage.

Other environments, like personal computers and Google Colaboratory[2], were also employed in different stages of this work, but their specifications were omitted because they were not directly used to produce the results presented in this Chapter.

Finally, for all tests executed on *Lobo Carneiro*, process orchestration was done through a software developed in Python and the allocation of processes to logical processors (threads) was ultimately done by the operating system. In other words, it was expected, for every instance execution, to run on a single system thread, with up to 48 executions running simultaneously. However, the end result depended on the operating system.

Additionally, the machine learning models used, when executed, may also create additional threads and processes, a situation the code used had little or no con-

[1]NACAD: <`https://portal.nacad.ufrj.br/`>.

[2]Google Colaboratory: <`https://colab.research.google.com/`>.

trol over. For those reasons, the times observed in this chapter should be taken cautiously. Under ideal conditions, where the executions and the machine learning models would run individually on dedicated hardware, better times are expected to be observed.

4.2 Evaluation on Unseen Instances

In this section the machine learning models are confronted with instances belonging to the same problems from where the instances used to train them belong to. In other words, given a model A, trained on a dataset belonging to an instance I_1 from a problem P_1, the results in this section focus on showing the error RMSE obtained when A is used to make predictions on datasets from other instances I_n, from that same problem P_1, where $I_1 \neq I_n$. Since those datasets are the eleven mentioned in Section 3.2, they are composed of 20 executions. However, the errors RMSE presented in this section are the average of the erros RMSE observed at each execution in a dataset or, in other words, for given a dataset from an instance I_n, composed of executions $E_1, ..., E_m$, where $m = 20$, the RMSE error presented is the result of Equation (4.1). In this work, that average RMSE is referred as $RMSE_{AVG}$.

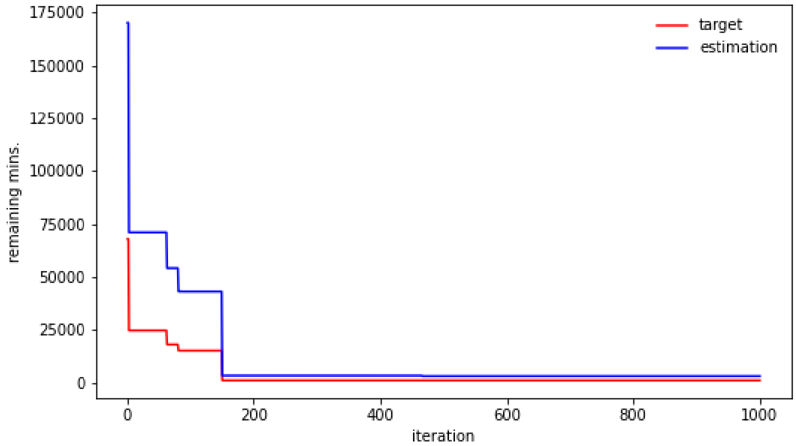
$$RMSE_{AVG} = \frac{(RMSE_{E_1} + ... + RMSE_{E_m})}{m} \tag{4.1}$$

It is also important to note that, as mentioned in Section 3.2.2, the target variable used by the models is the number of remaining minimums in future iterations. For that reason, the outputs are integers, instead of probabilities. Additionally, in all heatmaps in this section, the range used for the colors goes from 0 to 1000. The reason for that is the observation that, in general, a $RMSE_{AVG}$ of up to 800 tends to represent a *relatively good* fitting across the executions of a dataset, where *good* means that the error is tolerable and often better than or not too far off if compared to the one obtained through the method of RIBEIRO *et al.* [1].

More specifically, the reason for considering an error of such a magnitude as tolerable is mainly tied to the metric used, that is the root mean square error. That metric is highly sensitive to large deviations from the target due to the fact that those errors are squared. For that reason, if, at some iteration, a model estimates a number of remaining minimums that diverges significantly from the target value, that error will be squared and will be likely to impact the error calculated over the entire execution.

In the case of the behavior of the models produced in this work, large deviations from the target are something common at the first few hundred iterations and, in some cases, an erratic behavior can also be observed in that interval. After that, it is common for the estimates to get closer and closer to the target. To illustrate that, in Figure 4.1, for a decision tree regressor, trained on instance *scp42* using the features (*best_cost*, *best*), it is possible to see that, when a *scp55* execution is evaluated, there is a relevant deviation from the target at the first 200 iterations. However, that divergence gets smaller soon after that and, in the end, for the whole execution, the RMSE error is 486.92, showing that the model can be effectively used for that execution.

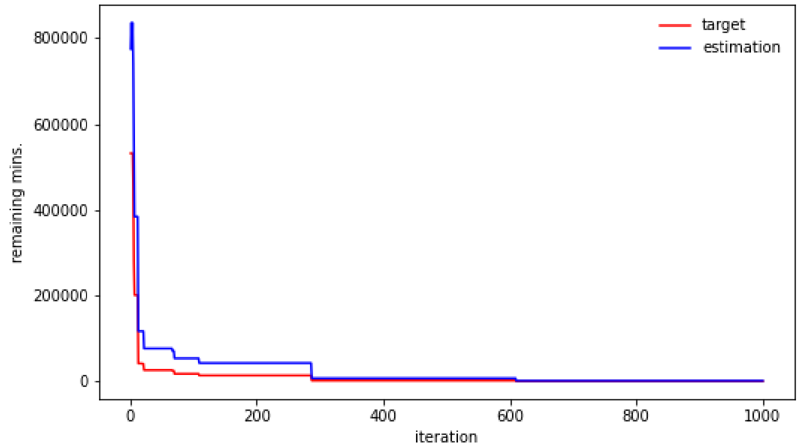
Figure 4.1: Fitting of the estimates of a decision tree regressor, trained on the *scp42* dataset using the features (*best_cost*, *best*), when evaluating the first 1 000 iterations of a *scp55* execution.



On the other hand, when another *scp55* execution is evaluated, a much bigger error can also be obtained. In Figure 4.2, the results for an execution generated with a seed different from the one used by the previous execution is shown. In that Figure, it is possible to see that, once again, in the first few hundred iterations, the deviation is significant. However, the difference is much more significant in the first 10 iterations, leading to a RMSE error of 984.67 for the whole execution. Despite that, if future iterations are observed, the model shows a better behavior, making it capable of effectively producing estimates for that execution. In the end, when the $RMSE_{AVG}$ for the *scp55* dataset (composed of 20 executions) is calculated, the error is 645.23, demonstrating that, while the error obtained on some executions might be higher than 800, that is usually caused by exceptionally high deviations in the first iterations, and not by an overall bad fitting.

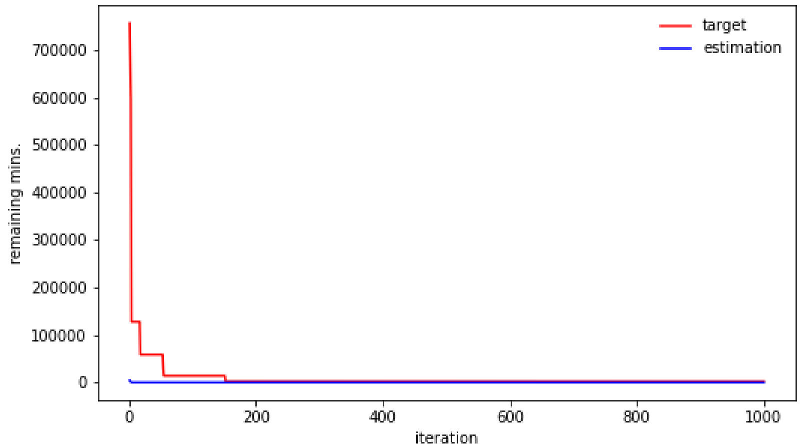
As for why the threshold between *good* and *bad* was defined as 800, it has to do with the cases where the models show poor performance on an entire dataset. Basically, it was observed that, usually, situations where an overall bad fitting occurs have a $RMSE_{AVG}$ greater than 1 000, because most of its executions will have a RMSE error higher that. For example, in Figure 4.3, the same *scp42* model is applied to a *scpb5* execution, but a poor fitting is obtained, leading to an overall RMSE error of 1324.97. If the entire dataset is taken into consideration, the $RMSE_{AVG}$ is

Figure 4.2: Fitting of the estimates of a decision tree regressor, trained on the *scp42* dataset using the features (*best_ cost*, *best*), when evaluating the first 1 000 iterations of a *scp55* execution.



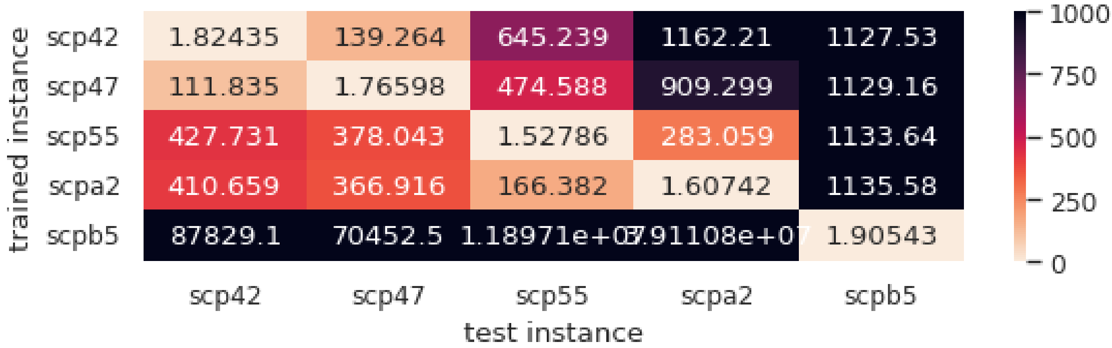
1127.53, and that happens because, in all executions, and for almost all iterations, the model estimates 0. However, in some cases, bad results can also be observed even in situations where the $RMSE_{AVG}$ is between 800 and 1 000, an interval where some *not so bad* results can also be found. In order to avoid that interval where the quality of the results is not so clear, it was decided to consider as *good* only $RMSE_{AVG}$ values inferior to 800.

Figure 4.3: Fitting of the estimates of a decision tree regressor, trained on the *scp42* dataset using the features (*best_ cost*, *best*), when evaluating the first 1 000 iterations of a *scpb5* execution.



With that said, in Figure 4.4, a heatmap showing the $RMSE_{AVG}$ obtained by Decision Tree Regressor models trained on SCP instances, using the features (*best_-cost*, *best*) (the ones with the highest correlation to the target variable), is shown. In that figure, it is possible to see that, for instances *scp42* and *scp47*, the error is low, showing that it is possible to use a model from one of them to predict the remaining minimums on another. It is also possible to see that the same applies *scp55*, but

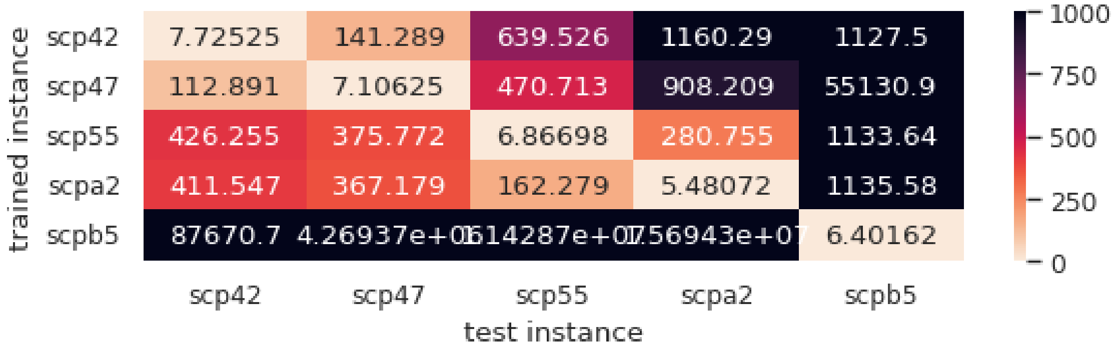
Figure 4.4: $RMSE_{AVG}$ for decision tree regressors, trained on SCP instances using features (*best_cost*, *best*), when evaluated on datasets from other SCP instances.



with a fitting not as good. When it comes the instance *scpa2*, the model trained on it showed a good performance when evaluted on the instances *scp42*, *scp47* and *scp55*, but the same did not happen when the models from *scp42* and *scp47* were evaluated on the *scpa2* dataset. In the same figure, the only instance whose model did not show any *compatibility* with any other instances was the *scpb5*.

If the type of model is changed to a Random Forest Regressor and the features are kept as (*best_cost*, *best*), it was also observed that the results are similar. In Figure 4.5, it is possible to see that, apart from some minor changes on $RMSE_{AVG}$, the *compatibility* between the instances stays the same.

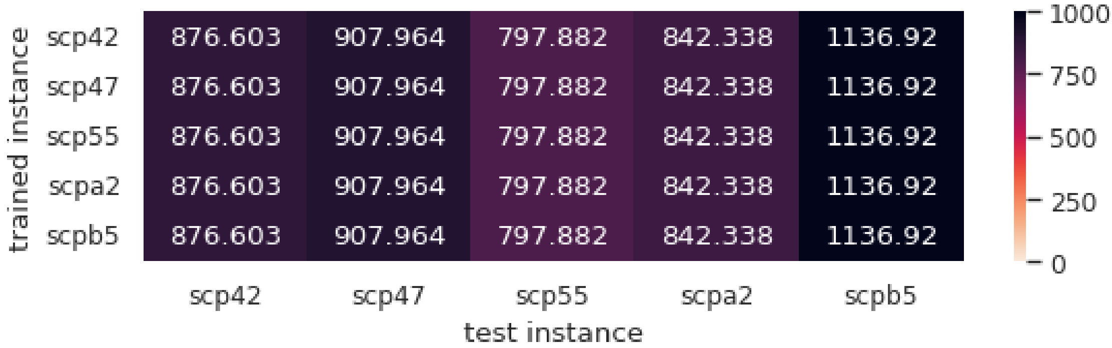
Figure 4.5: $RMSE_{AVG}$ for random forest regressors, trained on SCP instances using features (*best_cost*, *best*), when evaluated on datasets from other SCP instances.



When it comes to Extreme Gradient Boosting regressors, on the other hand, the situation is different. With the parameters defined in Section 3.4.3, Figure 4.6 shows that the models have a poor performance if compared to decision tree regressors and random forest regressors.

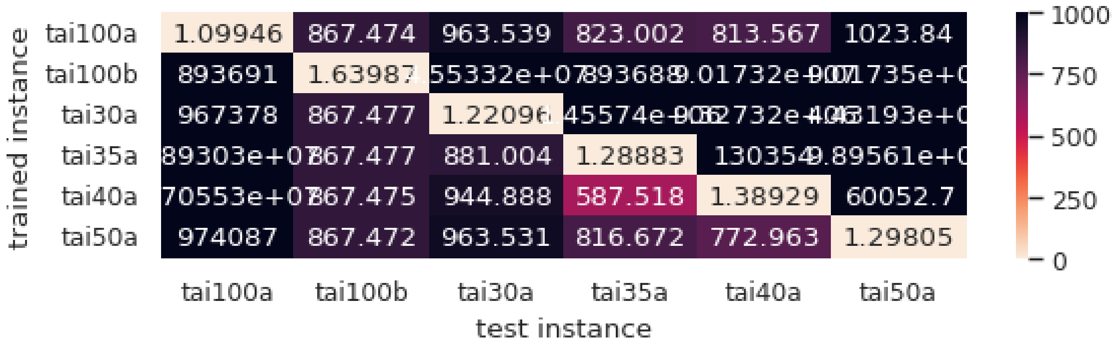
As for the results obtained by the decision tree models trained on QAP instances using the features (*best_cost*, *best*), Figure 4.7 shows that that feature combination

Figure 4.6: $RMSE_{AVG}$ for XGBoost regressors, trained on SCP instances using features (*best_ cost*, *best*), when evaluated on datasets from other SCP instances.



did not produce good results. The only case where any relevant compatibility was observed was in a *tai40a* model that was able to achive a relatively low $RMSE_{AVG}$ when evaluating a *tai35a* dataset. However, that occurrence was not reciprocal.

Figure 4.7: $RMSE_{AVG}$ for decision tree regressors, trained on QAP instances using features (*best_ cost*, *best*), when evaluated on datasets from other QAP instances.



When evaluating using random forest models, the results were similar to the ones obtained by the decision tree regressors, as shown in Figure 4.8. Figure 4.9 shows that the XGBoost regressors were also unable to achieve a desirable $RMSE_{AVG}$. That shows that that feature combination is not applicable for the QAP problem.

On the other hand, it is possible to argue that, for SCP instances, the feature combination (*best_ cost*, *best*) allows the creation of models that might be able to be successfully applied to a limited set of instances of that same problem. As for why that is possible, it is not clear. Based on Table A.1, it can be seen that the instances *scp42*, *scp47* and *scp55* have boundaries that are considerably similar. However, it is hard to point that as a deciding factor. One of the reasons for that is the fact that, while the instances *scpa2* and *scpb5* also have lower and upper bounds that are considerably similar, *scpa2* models can be used to predict remaining minimums on

Figure 4.8: $RMSE_{AVG}$ for random forest regressors, trained on QAP instances using features (*best_ cost*, *best*), when evaluated on datasets from other QAP instances.

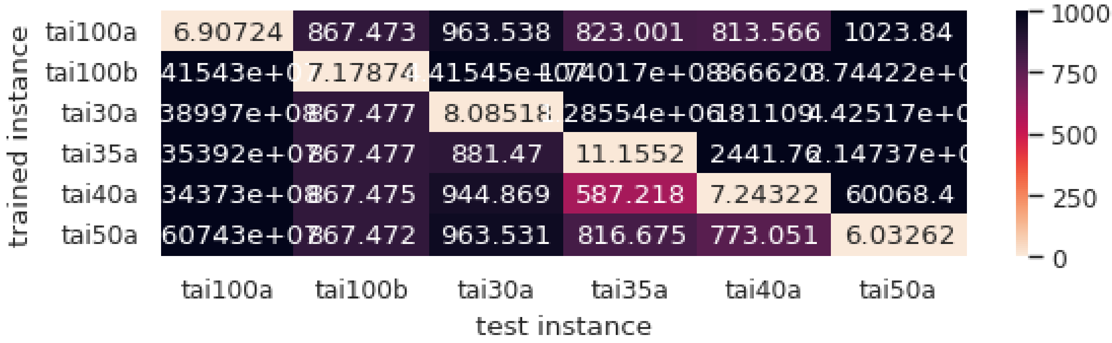
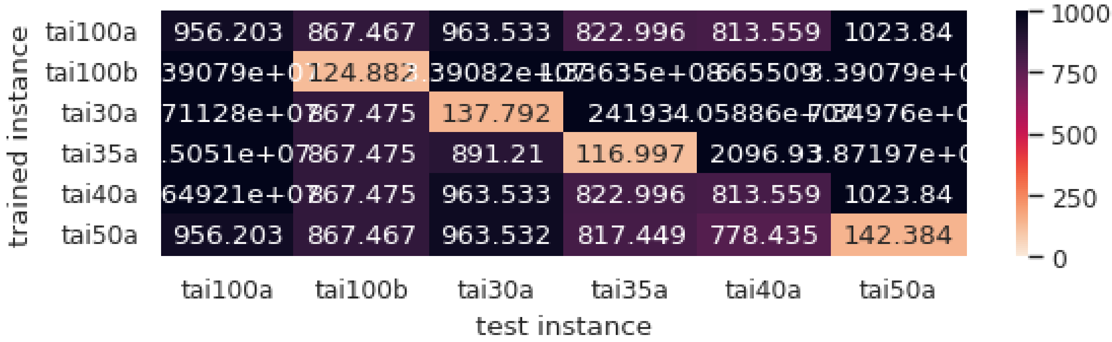


Figure 4.9: $RMSE_{AVG}$ for XGBoost regressors, trained on QAP instances using features (*best_ cost*, *best*), when evaluated on datasets from other QAP instances.



other datasets from other instances and *scpb5* models can not. This becomes even more evident in Section 4.3, where it is shown that some models might be useful even on data from other problems.

After showing the results for the feature combination composed by the features with the highest correlation with the target variable, another combination that must be considered is (*iteration*, *iterations_ since_ last_ min*, *iterations_ since_ best_ cost*, *total_ single_ mins_ found*). The reason for that is the fact that, at first, it was the one that seemed to present the highest generalization capabilities among those considered in this work. In Figures 4.10 and 4.11 it is possible to see that, regardless of problem, for any decision tree regressor trained on it, the $RMSE_{AVG}$ is always bellow 800. It is also evident that it came at a cost of having a higher in-sample $RMSE_{AVG}$.

When it comes to random forest regressors and XGBoost regressors, the situation is similar, as can be seen in Figures B.10 and B.15, respectively. Those two figures include SCP and QAP problems and will be revisited in Section 4.3.

In this section, the results for some feature combinations were not shown. How-

Figure 4.10: $RMSE_{AVG}$ for decision tree regressors, trained on SCP instances using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*), when evaluated on datasets from other SCP instances.

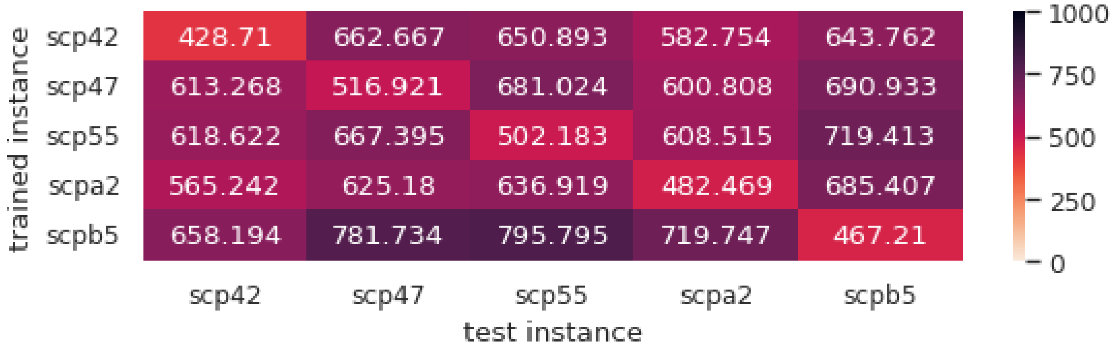


Figure 4.11: $RMSE_{AVG}$ for decision tree regressors, trained on QAP instances using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*), when evaluated on datasets from other QAP instances.

ever, they can be seen in Appendix B, where the heatmaps for all of them are available. Among those that are not present, the only ones that are worth mentioning are those employing the combination (*iteration*, *cost*, *best*), because the models trained on them showed a performance that can be placed between what is achieved by (*best_cost*, *best*) and (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*). That is evidenced by Figures B.3 and B.8.

4.3 Evaluation on Unseen Problems

In Section 4.2, the models showed promising results when evaluated on instances belonging to the problem that the instance they were trained on was taken from. In this section, the evaluation is expanded to other problems. In Figure 4.12, it is possible to see that, for decision tree regressors trained using the features (*best_cost*, *best*), a significant compatibility between instances of different problems is not observed. Some of the QAP models showed a $RMSE_{AVG}$ bellow 800, but very close to it, when evaluated on scp55 executions, making those results not very appealing. The same applies to decision tree regression models trained using the features (*iteration*, *cost*, *best_ cost*) and (*iteration*, *cost*, *best_ cost*, *best*), as can be seen in Figures B.2 and B.4.

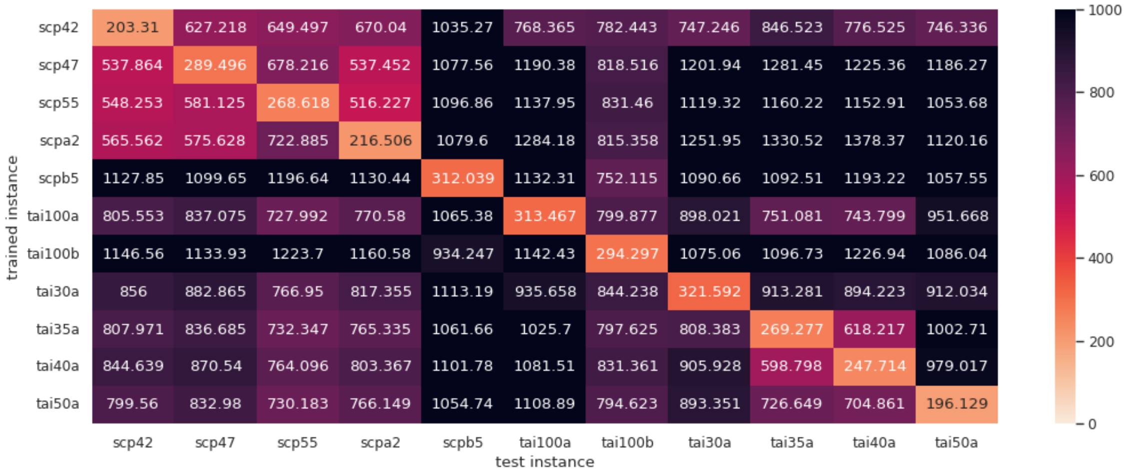
Figure 4.12: $RMSE_{AVG}$ for decision tree regressors, trained using features (*best_-cost*, *best*), when evaluated on datasets from different instances and problems.

When using the random forest regressors, the results are very similar to those obtained by the decision tree regressors, but with minor differences in error. That is evidenced by Figures B.6, B.7 and B.9. The XGBoost models, if trained using the features (*iteration*, *cost*, *best_ cost*, *best*), manage to show similar results to those obtained by the other regressors, as shown by Figure B.14. However, they fail to show any relevant intraproblem or interproblem compatibility when trained on the other two combinations, as can be seen in Figures B.11 and B.12.

As for the feature combinations (*iteration*, *cost*, *best*) and (*iteration*, *iterations_-since_ last_ min*, *iterations_ since_ best_ cost*, *total_ single_ mins_ found*), that is where the results become more interesting. For example, in figure 4.13, the decision tree regressor trained on a *scp42* instance using the features (*iteration*, *cost*, *best*) shows compatibility not only with multiple SCP instances, but also with multiple QAP instances. The same situation is observed for models trained on other instances. The problem is that the compatibility is not always reciprocal.

For that same set of features, compatibility across problems is also observed on random forest regressors, that show results similar to those obtained by the decision tree regressors, as can be seen in Figure B.8. On the other hand, the results obtained by the XGboost regressors are not promising, given the fact that it only showed error bellow 800 in few occasions, having poor results even on instances where those models were trained on, as shown by Figure B.13.

Figure 4.13: $RMSE_{AVG}$ for decision tree regressors, trained using features (*iteration*, *cost*, *best*), when evaluated on datasets from different instances and problems.



Lastly, the best results observed in the heat maps present in Appendix B were obtained by the set of features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*). Figure 4.14 shows that, through the use of XGBoost regressors trained using those features, it is possible to achieve intraproblem and interproblem compatibility with all instances present in it. Similar results are also obtained by the other regressors if those same features are used, as evidenced by Figures B.5 and B.10.

Figure 4.14: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*), when evaluated on datasets from different instances and problems.

Given those results, the next step is to see how a model trained with those features performs on more instances and how it compares to the estimator of RIBEIRO *et al.* [1], specifically the version where the normal distribution is truncated (the boundaries available are covered in Section 3.2.3). However, It is importance to note that, because of the differences in methodology mentioned in Section 3.2, the two techniques might not be directly comparable and, for that reason, any comparison present in this chapter should be taken cautiously.

With that said, in order to see how they perform, 20 instances were picked, where each problem was represented by 10 and each instance was composed of 10 executions of 1 000 000 iterations. As for the model, the XGBoost regressor trained on the instance *scp42* unsing the features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*) was chosen. The results are presented in Table 4.1.

Instance	Prob. Stop. $RMSE_{AVG}$	ML Stop. $RMSE_{AVG}$
scp42	1183.977	685.566
scp49	878.609	568.823
scp51	1039.964	564.044
scp65	1805.396	701.463
scp410	979.393	937.042
scpa4	828.858	664.459
scpb3	3509.505	547.835
scpc1	789.983	786.967
scpd1	3209.535	793.654
scpd5	3020.280	706.606

Instance	Prob. Stop. $RMSE_{AVG}$	ML Stop. $RMSE_{AVG}$
bur26d	444.061	3629.979
chr22a	941.914	1363.105
esc16j	1661.684	147175.093
had12	321.235	59845.361
lipa20a	562.791	6869.520
nug12	486.695	9922.096
rou20	385.643	960.119
sko56	802.080	805.096
tai30a	493.438	701.353
wil50	1532.034	649.188

Table 4.1: Error $RMSE_{AVG}$ for the XGboost model trained on scp42 instances using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*).

The values shown in that table demonstrate that the selected model performs well on SCP instances, achieving a $RMSE_{AVG}$ smaller than the ones obtained from the estimates provided by the estimator of RIBEIRO *et al.* [1]. On the other hand, when the results for the QAP instances are observed, it is possible to see that the regressor lost in many instances and even performed very poorly in some.

When the reasons for the bad performance on instances *bur26d*, *chr22a*, *esc16j*, *had12*, *lipa20a* and *nug12* are investigated, the first relevant information to be given is related to the method used to obtain those numbers, that was different for each problem. For the SCP instances, the estimates were calculated (1) at the first iteration, (2) at every time the best solution changed, and also (3) at every 50 iterations. Meanwhile, for the QAP instances, the calculation only happened in the first two situations.

That difference was motivated by the fact that, for the QAP problem, the estimator of RIBEIRO *et al.* [1] can take several minutes to calculate the CDF, while it can take up to a little more than a second to do the same for the SCP instances. That slowness is caused, among other factors, by the huge distances between the boundaries of some QAP instances, that are taken into account during the calculation of the integral.

It is also important to mention that, for the executions of the instances present in the table, the calculation of the RMSE for a single execution was performed over all iterations it has. To make that possible, iterations where the estimators were not executed received the estimates obtained at the last prior iteration where they were.

The second relevant information to be considered are the characteristics of the instances. In the case of the *esc16j*, the optimal solution is usually found in the first 10 iterations, while in *bur26d*, *had12*, *lipa20a* and *nug12* it appears within the first few hundred iterations. While this kind of event might be *identified* by models that take into account cost value, the same does not apply to the model employed, because it does not know the cost obtained at a given iteration and was trained on an instance where the solution is gradually improved over time.

Given that situation, if the XGBoost regressor is replaced by a model trained on a set of features that is aware of cost value, there might be room for improvement. In Table 4.2, the results obtained from a decision tree regressor trained on a scp42 instance using the features (*iteration*, *cost*, *best*) are presented.

Instance	**Prob. Stop.** $RMSE_{AVG}$	**ML Stop.** $RMSE_{AVG}$
scp42	1183.977	602.545
scp49	878.609	690.485
scp51	1039.964	361.297
scp65	1805.396	598.271
scp410	979.393	525.995
scpa4	828.858	358.393
scpb3	3509.505	755.885
scpc1	789.983	306.965
scpd1	3209.535	575.697
scpd5	3020.280	638.862

Instance	**Prob. Stop.** $RMSE_{AVG}$	**ML Stop.** $RMSE_{AVG}$
bur26d	444.061	1320.345
chr22a	941.914	640.586
esc16j	1661.684	38659.235
had12	321.235	13044.678
lipa20a	562.791	2699.114
nug12	486.695	10667.865
rou20	385.643	595.476
sko56	802.080	566.802
tai30a	493.438	888.368
wil50	1532.034	810.466

Table 4.2: Error $RMSE_{AVG}$ for the Decision Tree Regressor model trained on scp42 instances using features (*iteration*, *cost*, *best*).

Comparing those results to the ones shown in Table 4.2, it is possible to see that the use of the cost-aware features improved the results for many instances (while also increasing the error on a few others, but not by a very significant amount), resulting in a smaller error than the cost-unaware model, that, according to Figure 4.14, appeared to have better generalization capabilities. It also increased the number of situations where the machine learning model obtains a smaller error than the CDF-based estimator. Nonetheless, the errors continue to be high for the instances *bur26d*, *esc16j*, *had12*, *lipa20a* and *nug12*, and one of the few ways to reduce it further, without resorting to problem-specific models (like one trained on an easy QAP instance), may be through the production of estimates at fixed intervals, like what was done for the SCP instances.

In Table B.1, that approach is evaluated and validated on an extensive group of instances, where it can be seen that, by estimating the probability regularly, the error can be reduced. In that table, the models marked by (ii) produced estimates at the first iteration, every time the minimum changed and at every 50 iterations, while the estimators accompanied by a (i) were run in the first two situations.

In addition to the models used in Tables 4.1 and 4.2, Table B.1 also includes results for two *tai100a* estimators that were trained on the same feature sets used by the *scp42* models. However, despite the fact that those estimators also showed positive results when the probability is evaluated regularly, they did not seem to bring any relevant advantage when compared to their *scp42* counterparts (even on QAP instances), but it is important to note that the *tai100a* is not an easy instance and, unlike the *esc16j* or the *bur26d*, the optimal solution is not expected to be found after just a handful of iterations.

It is also possible to see that not all instances were represented by 10 executions. That happened because some executions experienced errors while running the estimator of RIBEIRO *et al.* [1] (in most cases, it appeared to be some kind of variable overflow) or while running GRASP (in few occasions, the program apparently crashed before reaching one million iterations). In some cases, that kind of problem also impeded the use of all executions of an instance. For instances *esc16b*, *esc16f*, *esc16h*, *esc16i*, *esc32e* and *esc32g*, all executions experienced errors (the one that appears to be a variable overflow) and, for that reason, their respective results were not included. Some instances were also removed due to their difficulty. Specifically, instances *tai150b*, *tai256c* and *tho150* were initially considered and some of their executions were started, but, due to the long time required to reach one million iterations, they were discarded.

With that said, in Table 4.3, a comparison between the CDF based estimator and the machine learning models is provided, based on the data available in Table B.1. In that table, the SCP problem is represented by 45 instances, while the QAP is represented by 125. It is possible to observe that, for a XGBoost regressor, trained on instance *scp42*, using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*), it is possible to obtain a smaller error than the estimator of RIBEIRO *et al.* [1] in more than 50% of the instances, in both problems. But that only happens if the estimates are produced at every 50 iterations and are compared to the CDF being executed only at iterations where there is a change in minimum. If both techniques produce estimates only during minimum changes, the machine learning models still show better results on SCP instances, but perform worse than the CDF in QAP instances. In any case, it is important to note that those results must be taken cautiously, given the difference in methodology (mentioned in Chapter 3) between the present work and the work of RIBEIRO *et al.* [1].

model	**estimation moment**	**% model smaller error (all inst.)**	**% model smaller error (SCP inst.)**	**% model smaller error (QAP inst.)**
XGB_E_scp42	(i)	40.0	84.4	24.0
XGB_E_scp42	(ii)	68.8	100.0	57.6
DTR_C_scp42	(i)	40.6	93.3	21.6
DTR_C_scp42	(ii)	58.2	100.0	43.2
XGB_E_tai100a	(i)	33.5	84.4	15.2
XGB_E_tai100a	(ii)	65.9	100.0	53.6
RFR_C_tai100a	(i)	44.1	100.0	24.0
RFR_C_tai100a	(ii)	59.4	100.0	44.8

Table 4.3: Comparison between the CDF-based estimator and four machine learning models when evaluating 170 different instances (45 SCP and 125 QAP). In all cases, the CDF-based estimator was only executed in the first iteration of an execution and during minimum changes.

Another important aspect to be evaluated in this work is the time an estimator takes to output a value. In Table C.1, the average times obtained while running the instances presented in Tables 4.1 and 4.2 are presented. Based on those results, it is possible to argue that the machine learning based approach can be faster than the CDF-based estimator. However, the time taken depends on the machine learning technique being utilized. When the times observed for the XGBoost regressor are compared to those observed for the decision tree regressor, the latter proves be much faster than the former, and that is caused by the fact that a decision tree regressor is much simpler than a XGBosst regressor, as shown in Sections 2.2.1 and 2.2.3.

Lastly, in Table C.2 the stopping rule is evaluated. Specifically, it is observed at which iteration executions of the instances present in Table C.1 would stop, given a threshold β. In those results, it is possible to observe, in a more practical way, how well the XGBoost regressor and the decision tree regressor perform on SCP and QAP instances. It corroborates, for example, with the argument that the machine learning models utilized have a bad performance on easy QAP instances and that the estimation of the probabilities at fixed intervals could have improved that situations.

4.4 Model Choice

In this work, a total of 165 models were generated and utilized for testing purposes. Most of them were only applied to a limited set of unknown instances, while a few others were used to make predictions for many more. In that universe of models, they varied on instance used for training, machine learning technique and feature set, and that leads to one question: which one should be used?

The answer for such a question is not simple. Considering the results obtained in this work, two feature sets showed relevant generalization capabilities. They are (*iteration*, *cost*, *best*) and (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*). However, the features are only part of the decision process. The machine learning technique and the parameters used by them are also of utmost importance. To exemplify that, the results obtained by the XGBoost regressor for most feature combination can be used. The technique itself is expected to be more powerful than decision tree regression and random forest regression. Nonetheless, it achieved bad results in many scenarios because of an apparently poor parameter selection.

Based on those facts, the recommendations made by this work are not limited to a single model, technique, etc. If simplicity and very fast training speeds are important, decision tree regression has shown to be as usable as the other two techniques. On the other hand, if less risk of over fitting is desired, random forest regression and XGBoost might be a good choices.

Additionally, as mentioned earlier, two feature sets showed relevant results. However, instead of considering only one of them, the use of both might be a better choice, because one showed better results on some instances, while the other was better on others. In that case, two models could be used, forming an ensemble where each of its components would be trained using a different feature set. The output, in that case, could be the average or the smallest probability estimated among the models.

When it comes to which instance should be used for training, it depends on the target problem and instance. In the context of this work, models trained on a *scp42* showed good results when used to evaluate other SCP instances, but faced a less favorable scenario in QAP instances, having a bad performance on easy ones. In those cases, the models would eventually stop the execution at some point, but possibly at a greater cost than the required by the estimator of RIBEIRO *et al.* [1].

Chapter 5

Conclusions

This chapter closes this text by presenting the final remarks and a series of possible paths to be followed from the point where this work stopped.

5.1 Final Remarks

In this work, it was shown that machine learning can be used to replace the role performed by the CDF in the probabilistic stopping rule for the GRASP metaheuristic. With the approach taken, it was possible to achieve a better performance on many of the instances tested, and that happened for the time required to evaluate an iteration and for the error obtained by the estimates when they are compared to the expected values within sufficiently large executions (large samples).

Moreover, the method also demonstrated generalization capabilities, where some models trained on a given instance of a given problem were able to provide relevant estimates for executions from instances belonging to the same problem and to other problems. The key in this case resides in the features used by the models. For example, models unaware of cost value might be able to generalize to more instances, while models trained on features that include cost value might produce better estimates on situations where the global minimum — or a very good local minimum — is found early in an execution, because that feature is able to express, indirectly, that the optimal solution (or a very good one) was indeed found.

The main drawback of the proposed technique, on the other hand, is the need to train a model before using it, which involves two time consuming activities. The first is data acquisition, that requires the accumulation of large executions of a given instance, and the second is the act of training the model on that data. Model training is usually the fastest part among the two. However, how long it takes depends on the machine learning technique being used.

In order to mitigate that, in this work, it was shown that tree-based models were fast to train, making the time required for that relatively negligible. As for the time required to obtain the training data, it still represents the main disadvantage of what is proposed in this work when compared to the stopping rule using CDF, that can work with any standard GRASP optimization without needing prior procedures. However, if the model proves to be able to generalize to the instances it is intended to be applied, the training will be a one-time activity.

Finally, it is possible to conclude that a machine learning based probabilistic stopping criterion for GRASP is feasible and effective, performing better than the original probabilistic stopping rule in many situations. But that comes at cost in time prior to its use that must be must be taken into consideration by those intending to use it. For that reason, the observations that can be made are that the stopping rule of RIBEIRO *et al.* [1] is more appropriate to situations where the time required to apply the method proposed in this work is not available and guaranteed generalization is needed, while the machine learning-based approach is more suitable to cases where the estimates are expected to be produced repeatedly in a short period of time.

5.2 Future Works

In order to expand the current work and possibly improve its results, six additional approaches are intended to be evaluated. The first is to verify the impact of aligning the methodology of the proposed technique to what is done by the stopping rule of RIBEIRO *et al.* [1] to calculate the number of future minimums. In this case, datasets of 2 000 000 iterations could be used, where iterations from 1 000 001 to 2 000 000 would be employed exclusively for that purpose, allowing the observation of 1 000 000 iterations in the future for any of the first 1 000 000 iterations.

As for the second future work, it would be checking the impact of tightening the boundaries of the instances. The upper bounds used in the present work were very loose and far from what was effectively observed in the executions, a fact that also contributed to the high times observed during the execution of the stopping criterion of RIBEIRO *et al.* [1] on QAP instances.

The third open possibility is to seek for ideal sizes for the dataset. The one employed in this work was based on limited tests and it might be possible to achieve similar results with datasets that are smaller (in number of executions or in number of iterations per execution).

The fourth possible approach is to check if online learning can be used somehow. The application of a machine learning technique of that kind could happen in combination with a traditional stopping criterion, like a limited number of iterations or time, where it could take over the decision process on whether to stop the search or not once it starts producing results as good as the other criteria. Similarly, the model could also be combined with the original probabilistic stopping rule and trained on its estimates. In these cases, the model might not produced better estimates, but might achieve results that are comparable to the other technique in a faster way.

The fifth loose end is the application of the method on other problems. In RIBEIRO *et al.* [1], four problems were used to test the technique they proposed, while, in this work, only two were employed. Testing the machine learning based approach on more problems would allow the identification of eventual additional limitations to its generalization capability.

The sixth - and last - thing that is intended to be evaluated in the future is the use of additional features and additional combinations of them. In this work, for example, cost autocorrelation and features derived from cost history (like average, variance and standard deviation) were not considered, but could produce relevant results.

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Appendix A

Instance's Lower and Upper Bounds

Instance	LB	UB	Instance	LB	UB
scp41	1148	37742	scp64	292	39068
scp410	1356	37151	scp65	353	39155
scp42	1205	37132	scpa1	562	58870
scp43	1213	37221	scpa2	560	58550
scp44	1185	37145	scpa3	524	58771
scp45	1266	37271	scpa4	527	58751
scp46	1349	37239	scpa5	557	58754
scp47	1115	36570	scpb1	149	59578
scp48	1225	37276	scpb2	150	59554
scp49	1485	37221	scpb3	165	59585
scp51	579	39087	scpb4	157	59740
scp510	672	38823	scpb5	151	59676
scp52	677	38818	scpc1	514	79004
scp53	574	38776	scpc2	483	79028
scp54	582	38736	scpc3	544	78796
scp55	550	38972	scpc4	484	78793
scp56	560	38911	scpc5	488	78697
scp57	695	38690	scpd1	122	79771
scp58	662	38341	scpd2	127	79714
scp59	687	38610	scpd3	138	79783
scp61	283	39344	scpd4	122	79520
scp62	302	38938	scpd5	130	79672
scp63	313	38895			

Table A.1: SCP instances and their respective lower and upper bounds.

Instance	LB	UB	Instance	LB	UB	Instance	LB	UB
bur26a	5426670	100245444	had18	5358	25056	sko100d	141289	1584000
bur26b	3817852	67331030	had20	6922	34280	sko100e	140893	1584000
bur26c	5426795	83306912	kra30a	88900	1326000	sko100f	140691	1584000
bur26d	3821225	55973502	kra30b	91420	1362000	sko42	14934	168840
bur26e	5386879	93811198	kra32	88700	1546240	sko49	22004	251860
bur26f	3782044	63025638	lipa20a	3683	14360	sko56	32610	358400
bur26g	10117172	187561244	lipa20b	27076	138400	sko64	45736	504320
bur26h	7098658	125978580	lipa30a	13178	50400	sko72	62691	682560
chr12a	9552	867240	lipa30b	151426	739620	sko81	86072	920970
chr12b	9742	867240	lipa40a	31538	118720	sko90	109030	1209600
chr12c	11156	867240	lipa40b	476581	2340240	ste36a	9526	862056
chr15a	9896	1529310	lipa50a	62093	234500	ste36b	15852	5799600
chr15b	7990	1529310	lipa50b	1210244	5801600	ste36c	8239110	700694568
chr15c	9504	1529310	lipa60a	107218	404940	tai100a	15844731	97714200
chr18a	11098	2212164	lipa60b	2520135	12043080	tai100b	1058131796	130115042000
chr18b	1534	140616	lipa70a	169755	650650	tai12a	224416	1256808
chr20a	2192	283320	lipa70b	4603200	22604400	tai12b	39464925	1757709624
chr20b	2298	283320	lipa80a	253195	970400	tai150b	441786736	26078235600
chr20c	14142	3021520	lipa80b	7763962	38504960	tai15a	388214	1935390
chr22a	6156	791604	lipa90a	360630	1395000	tai15b	51765268	12248023585
chr22b	6194	791604	lipa90b	12490441	62360910	tai17a	491812	2552635
chr25a	3796	1055650	nug12	578	5856	tai20a	703482	3626400
els19	17212548	1704030732	nug14	1014	10080	tai20b	122455319	13048373980
esc128	64	96768	nug15	1150	11850	tai256c	43849646	6553600000
esc16a	68	1632	nug16a	1610	14720	tai25a	1167256	5883300
esc16b	292	1728	nug16b	1240	13440	tai25b	344355646	28051179500
esc16c	160	2688	nug17	1732	16830	tai30a	1706855	8596620
esc16d	16	960	nug18	1930	18720	tai30b	637117113	42004266660
esc16e	28	1344	nug20	2570	24800	tai35a	2216627	11803330
esc16f	0	0	nug21	2438	31500	tai35b	242172800	20629796495
esc16g	26	1536	nug22	3596	47960	tai40a	2843274	15469120
esc16h	996	16128	nug24	3488	40320	tai40b	564428353	34766639600
esc16i	14	1632	nug25	3744	43500	tai50a	4390920	24275700
esc16j	8	864	nug27	5234	64800	tai50b	395543467	30319229200
esc32a	130	13568	nug28	5166	61600	tai60a	5578356	34999680
esc32b	168	8192	nug30	6124	70200	tai60b	542376603	49191714900
esc32c	642	16896	rou12	235528	1290840	tai64c	1855928	409600000
esc32d	200	8704	rou15	354210	2053350	tai80a	10501941	62394560
esc32e	2	4096	rou20	725522	3714560	tai80b	717907288	65951742240
esc32g	6	3584	scr12	31410	961560	tho150	8133398	114180600
esc32h	438	11776	scr15	51140	1858350	tho30	149936	2101860
esc64a	116	22400	scr20	110030	4897200	tho40	240516	3730400
had12	1652	7320	sko100a	143846	1584000	wil100	273038	1425600
had14	2724	13216	sko100b	145522	1584000	wil50	48816	258300
had16	3720	17408	sko100c	139881	1584000			

Table A.2: QAP instances and their respective lower and upper bounds.

Appendix B

Error Heatmaps and Error Tables

Figure B.1: $RMSE_{AVG}$ for decision tree regressors, trained using features (*best_-cost*, *best*), when evaluated on datasets from different instances and problems.

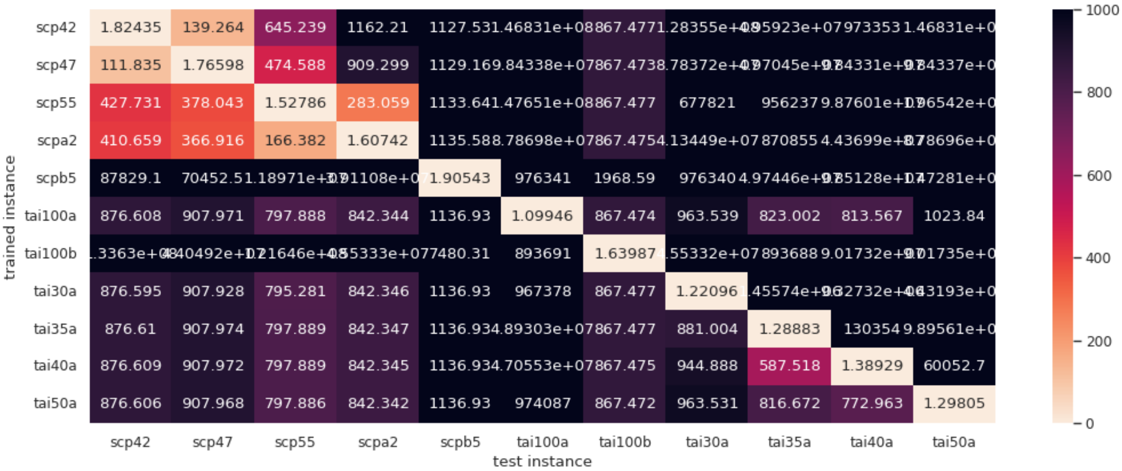

Figure B.2: $RMSE_{AVG}$ for decision tree regressors, trained using features (*iteration*, *cost*, *best_ cost*), when evaluated on datasets from different instances and problems.

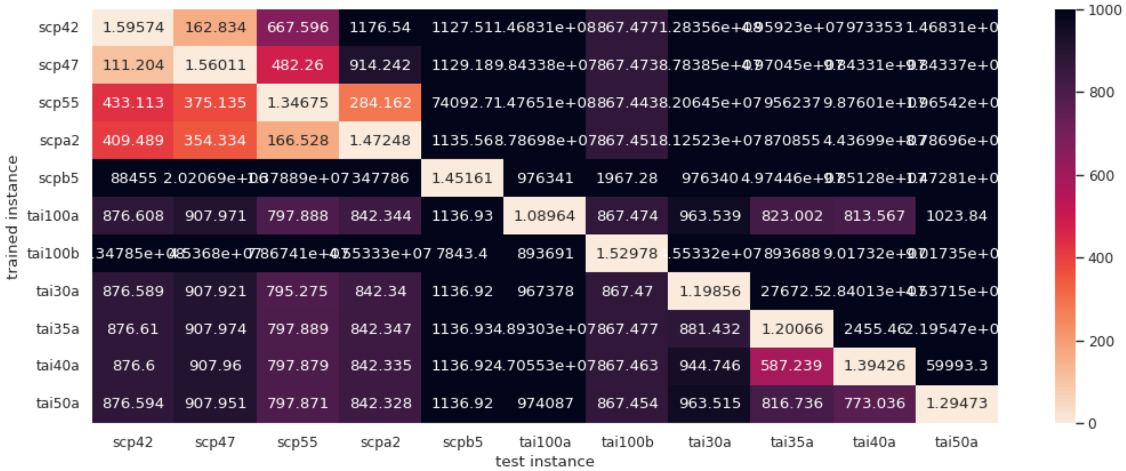

Figure B.3: $RMSE_{AVG}$ for decision tree regressors, trained using features (*iteration*, *cost*, *best*), when evaluated on datasets from different instances and problems.

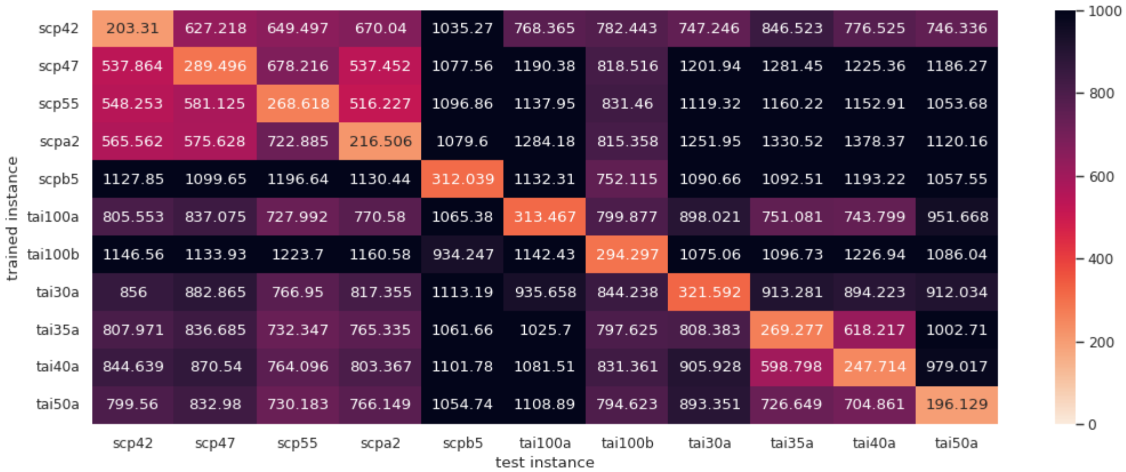

Figure B.4: $RMSE_{AVG}$ for decision tree regressors, trained using features (*iteration*, *cost*, *best_cost*, *best*), when evaluated on datasets from different instances and problems.

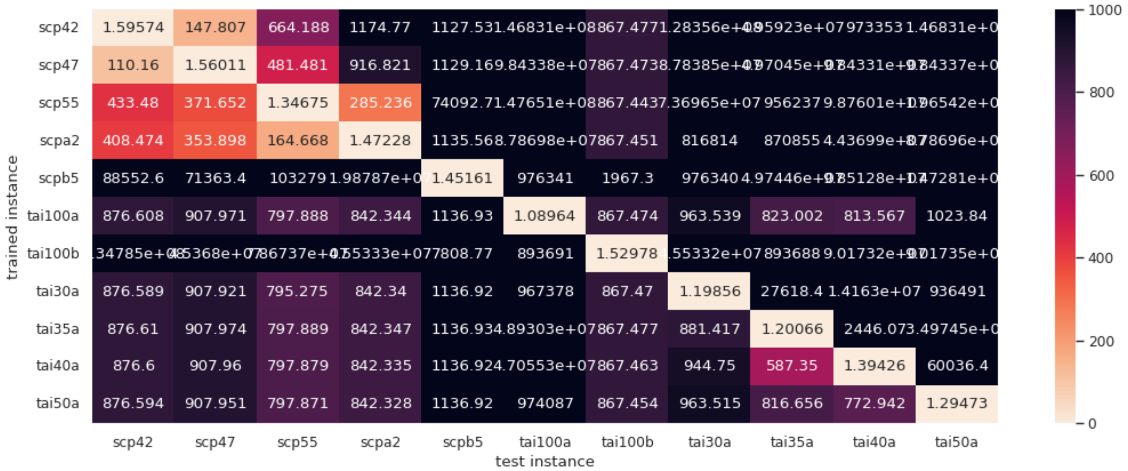

Figure B.5: $RMSE_{AVG}$ for decision tree regressors, trained using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_-found*), when evaluated on datasets from different instances and problems.

Figure B.6: $RMSE_{AVG}$ for random forest regressors, trained using features (*best_-cost*, *best*), when evaluated on datasets from different instances and problems.

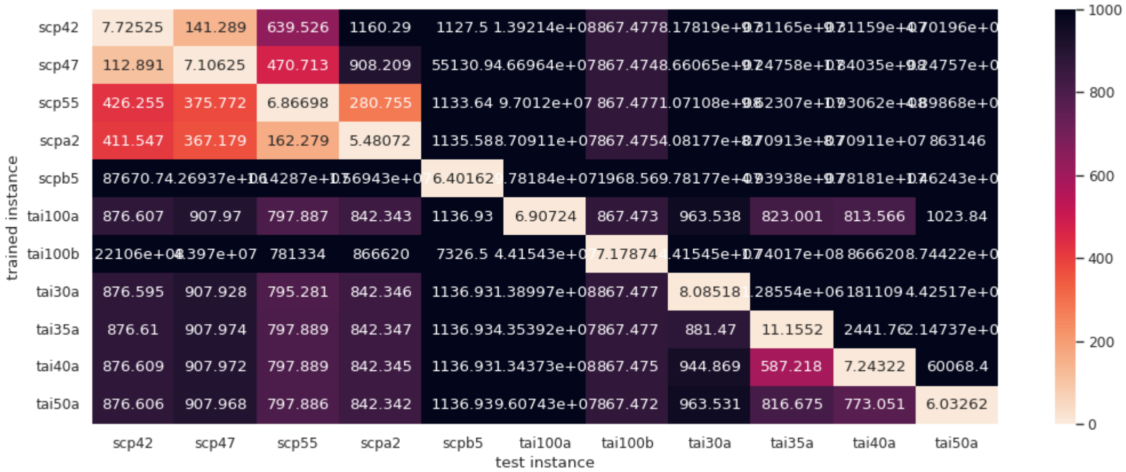

Figure B.7: $RMSE_{AVG}$ for random forest regressors, trained using features (*iteration*, *cost*, *best_cost*), when evaluated on datasets from different instances and problems.

Figure B.8: $RMSE_{AVG}$ for random forest regressors, trained using features (*iteration*, *cost*, *best*), when evaluated on datasets from different instances and problems.

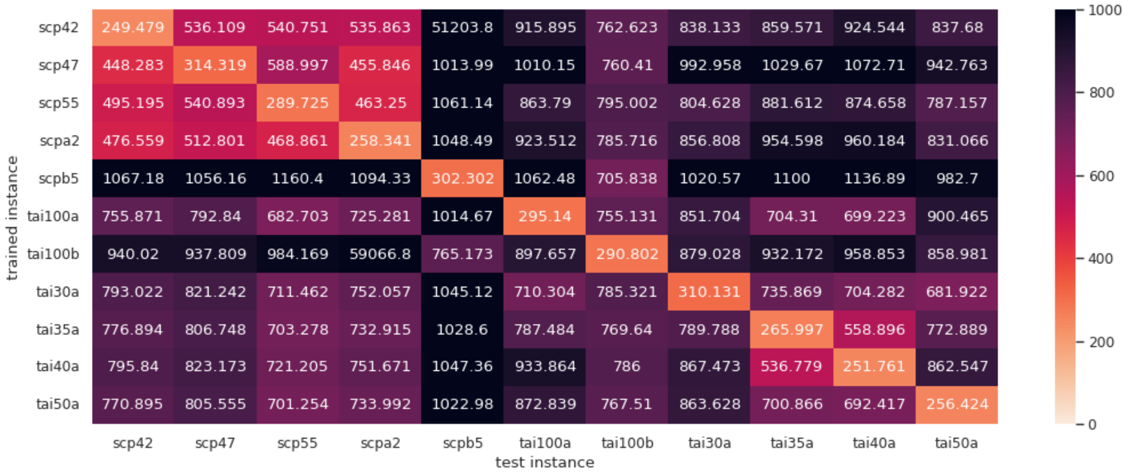

Figure B.9: $RMSE_{AVG}$ for random forest regressors, trained using features (*iteration*, *cost*, *best_cost*, *best*), when evaluated on datasets from different instances and problems.

Figure B.10: $RMSE_{AVG}$ for random forest regressors, trained using features (*iteration*, *iterations_since_last_min*, *iterations_since_best_cost*, *total_single_mins_found*), when evaluated on datasets from different instances and problems.

Figure B.11: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*best_cost*, *best*), when evaluated on datasets from different instances and problems.

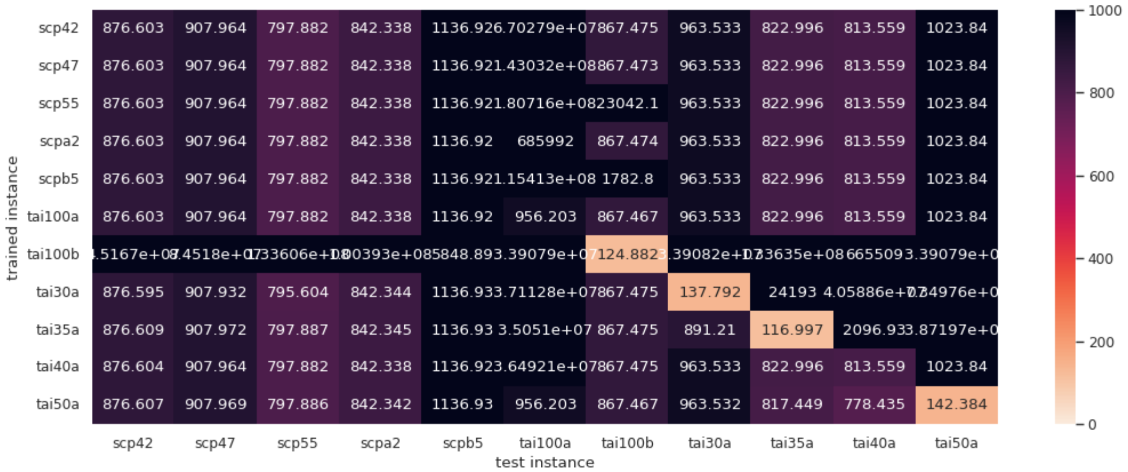

Figure B.12: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*iteration*, *cost*, *best_ cost*), when evaluated on datasets from different instances and problems.

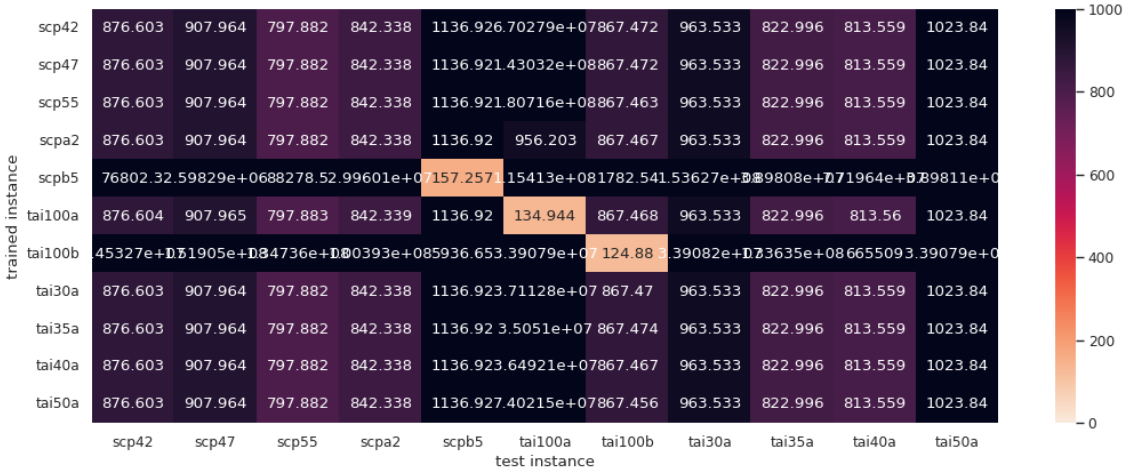

Figure B.13: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*iteration*, *cost*, *best*), when evaluated on datasets from different instances and problems.

Figure B.14: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*iteration*, *cost*, *best_ cost*, *best*), when evaluated on datasets from different instances and problems.

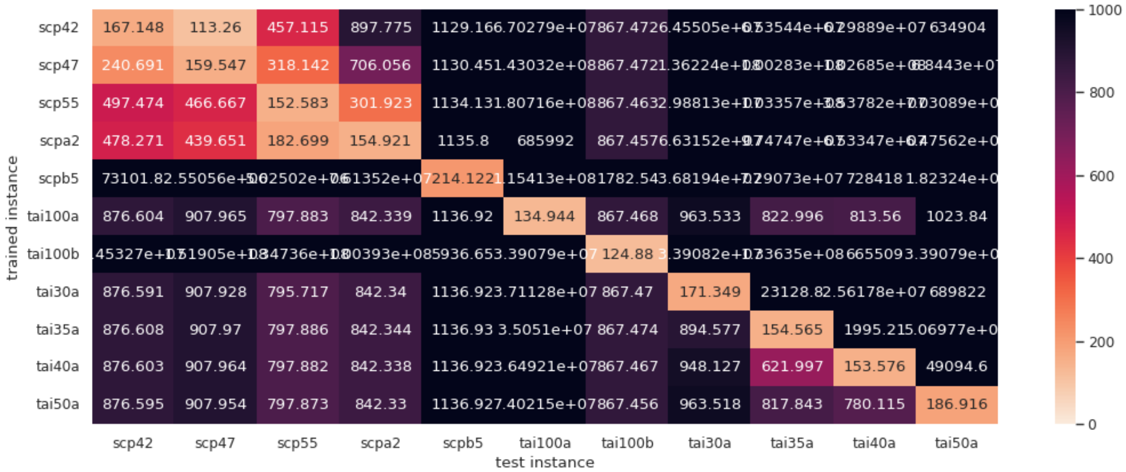

Figure B.15: $RMSE_{AVG}$ for XGBoost regressors, trained using features (*iteration*, *iterations_ since_ last_ min*, *iterations_ since_ best_ cost*, *total_ single_ mins_ found*), when evaluated on datasets from different instances and problems.

Table B.1: $RMSE_{AVG}$ observed for the probabilistic stopping rule of RIBEIRO *et al.* [1] and for different machine learning models when applied to multiple SCP and QAP instances. (i) are results obtained when the estimators are executed only in the first iteration and on changes of minimum cost, while in (ii) the estimators are also executed at every 50 iterations. Feature set codes come from Table 3.6.

Instance	**Num. (Execs.)**	**Prob. Stop (i)**	**XGB E scp42 (i)**	**XGB E scp42 (ii)**	**DTR C scp42 (i)**	**DTR C scp42 (ii)**	**XGB E tai100a (i)**	**XGB E tai100a (ii)**	**RFR C tai100a (i)**	**RFR C tai100a (ii)**
bur26a.dat	10	580.4	6296.1	627.4	3721.1	785.9	5615.0	632.3	5618.2	765.1
bur26b.dat	10	511.1	1839.0	793.8	1200.3	620.1	2871.7	573.3	1705.4	614.8
bur26c.dat	10	621.6	6940.1	683.2	3815.7	836.8	1525.7	741.2	4204.6	812.8
bur26d.dat	10	522.3	3133.8	665.1	2003.3	649.6	2071.1	570.6	3901.2	625.8
bur26e.dat	10	582.4	2728.1	565.7	1486.3	732.0	2044.7	706.8	1497.5	711.0
bur26f.dat	10	570.1	10173.5	452.3	5666.6	695.4	7623.8	549.4	5481.0	676.0
bur26g.dat	10	723.0	2084.3	726.3	2310.4	873.5	2046.4	687.0	1500.9	862.6
bur26h.dat	10	401.6	3549.2	540.6	2186.8	551.3	2405.7	442.9	4444.8	530.2
chr12a.dat	10	380.2	10719.4	498.7	5964.0	498.1	1937.7	521.6	7524.4	518.6
chr12b.dat	10	466.6	18423.1	775.4	11132.1	647.5	45341.9	647.6	18090.6	712.2
chr12c.dat	10	394.1	2195.1	401.0	1665.9	606.7	1651.4	443.3	2028.3	619.5
chr15a.dat	10	434.5	561.4	640.2	896.6	520.9	1768.3	535.9	1251.6	489.8
chr15b.dat	10	812.9	7595.9	737.1	3989.7	898.9	1292.5	777.7	4516.4	876.7
chr15c.dat	10	731.9	796.2	689.4	1563.1	725.7	1591.2	714.1	1582.3	717.7
chr18a.dat	10	498.5	826.0	474.2	910.4	755.4	862.3	507.7	1312.6	736.0
chr18b.dat	10	615.1	544.5	556.3	1691.2	543.4	21887.1	784.3	6018.5	526.0
chr20a.dat	10	758.5	902.1	691.2	887.2	847.9	902.1	694.5	1747.0	835.2
chr20b.dat	10	1172.2	892.7	600.1	1045.5	968.7	1055.3	649.3	1012.1	952.1
chr20c.dat	10	397.8	2282.1	439.4	1844.5	379.3	429.1	400.6	1105.4	356.8
chr22a.dat	10	765.9	914.2	693.9	722.6	730.8	714.1	582.8	713.6	708.7
chr22b.dat	9	675.2	647.5	491.1	607.1	613.0	782.7	477.2	576.3	584.8
chr25a.dat	10	661.5	963.1	615.3	803.4	783.5	785.4	636.5	816.2	762.7
els19.dat	10	947.5	10962.8	592.0	3456.3	517.1	16563.1	719.3	6260.3	482.7
esc128.dat	10	285.3	31618.0	408.4	6310.5	469.6	4860.6	545.6	9310.5	453.0
esc16a.dat	8	1244.5	244.0	753.6	29284.2	307.5	242317.2	964.7	21699.2	320.6
esc16c.dat	7	1063.1	90.8	677.6	38658.6	169.7	231606.6	867.1	25915.2	193.1
esc16d.dat	6	2016.7	0.0	687.3	38658.0	104.4	203941.7	615.6	24457.0	124.5
esc16e.dat	8	1591.3	69655.4	824.5	38658.4	161.2	169219.2	745.9	27007.9	184.6
esc16g.dat	9	1716.4	139621.2	806.2	34477.5	243.8	164843.3	830.3	26369.6	265.0
esc16j.dat	10	1777.8	91.5	696.5	34903.5	175.7	30881.5	1079.3	25469.2	198.6

Instance	Num. (Execs.)	Prob. Stop (i)	XGB E scp42 (i)	XGB E scp42 (ii)	DTR C scp42 (i)	DTR C scp42 (ii)	XGB E tai100a (i)	XGB E tai100a (ii)	RFR C tai100a (i)	RFR C tai100a (ii)
esc32a.dat	9	439.5	636.0	421.4	571.4	591.3	771.1	497.3	561.7	563.1
esc32b.dat	9	562.4	728.3	585.7	8984.9	347.1	27404.2	553.7	8287.3	334.6
esc32c.dat	6	1134.5	562.3	998.6	26263.6	589.5	158391.3	844.6	26705.6	600.8
esc32d.dat	10	305.2	3190.3	614.7	16571.1	448.3	75075.8	562.9	18854.2	446.4
esc32h.dat	9	380.4	11004.0	730.6	3171.2	340.9	7636.9	537.9	5275.0	323.0
esc64a.dat	5	2078.6	106303.5	856.8	38659.0	203.5	225889.1	888.4	25875.2	226.8
had12.dat	10	316.2	12338.7	500.8	3307.3	451.1	29262.3	451.0	11994.9	510.1
had14.dat	10	396.2	9894.1	512.4	35483.0	574.2	97662.7	650.7	17815.5	554.6
had16.dat	10	316.4	392.4	631.6	12181.2	422.3	114064.4	632.7	13871.9	382.5
had18.dat	10	355.5	16989.3	452.2	14757.2	616.4	13957.2	572.6	12868.4	607.0
had20.dat	10	446.3	6792.3	464.5	9435.8	657.3	11922.2	515.1	12409.4	650.3
kra30a.dat	10	850.4	1095.7	723.9	1474.1	585.8	952.1	583.8	1234.9	606.6
kra30b.dat	10	549.6	816.2	456.3	501.7	444.2	994.8	534.6	461.6	422.7
kra32.dat	10	593.0	854.8	496.3	1063.7	686.7	726.5	590.0	3008.6	665.5
lipa20a.dat	10	706.0	2802.9	534.4	7680.4	520.6	13434.9	654.5	6385.5	554.7
lipa20b.dat	10	414.2	24685.0	665.6	16577.0	523.9	66488.5	589.8	21588.0	692.3
lipa30a.dat	10	522.5	679.2	590.0	1611.3	581.3	1625.0	513.1	1150.2	608.6
lipa30b.dat	10	302.6	7429.1	521.7	10916.9	454.6	66177.6	487.3	15762.1	523.9
lipa40a.dat	10	609.8	605.4	565.9	623.6	626.1	847.3	557.2	608.9	620.5
lipa40b.dat	10	448.8	33470.7	516.6	37984.5	564.6	18189.8	617.1	10895.5	586.4
lipa50a.dat	10	563.8	603.3	537.9	647.3	654.2	641.9	560.1	680.1	647.9
lipa50b.dat	10	557.0	7624.8	626.1	3527.8	561.6	3946.5	606.4	3667.7	670.7
lipa60a.dat	10	513.3	863.0	509.6	1139.5	622.3	1158.0	496.3	1156.2	605.9
lipa60b.dat	10	335.1	4686.4	413.5	1368.0	583.8	10010.3	476.2	4383.7	503.8
lipa70a.dat	10	543.5	796.6	594.2	825.2	858.8	925.5	661.0	889.3	830.1
lipa70b.dat	10	641.0	4187.1	535.2	2606.0	591.7	9392.4	594.5	3582.4	571.7
lipa80a.dat	10	710.5	592.7	550.5	601.7	556.6	586.2	571.7	597.8	543.4
lipa80b.dat	10	509.1	821.3	589.8	1462.6	659.7	1509.5	625.9	1366.0	761.2
lipa90a.dat	10	701.7	833.0	621.0	782.7	795.3	957.5	679.7	759.5	764.4
lipa90b.dat	10	653.3	613.4	621.4	4524.5	575.7	2594.8	631.8	2389.0	545.3
nug12.dat	10	543.3	14305.4	689.0	7631.5	799.8	6292.9	636.0	8369.4	812.6
nug14.dat	10	406.8	3923.6	580.4	2501.1	652.6	2160.5	536.2	3074.7	702.8
nug15.dat	10	402.6	23567.3	556.7	3701.7	689.1	19548.3	531.2	11221.6	692.6
nug16a.dat	10	462.0	3890.4	412.4	1410.7	526.0	12041.1	478.1	2150.0	528.4
nug16b.dat	10	401.6	37224.7	449.3	7763.2	523.0	47965.9	647.7	14214.3	525.6
nug17.dat	10	551.8	1110.0	579.6	912.4	552.2	2433.0	663.1	1194.3	529.7
nug18.dat	10	417.5	618.0	478.0	5656.4	552.4	19568.3	507.5	4795.1	554.8

Instance	Num. (Execs.)	Prob. Stop (i)	XGB E scp42 (i)	XGB E scp42 (ii)	DTR C scp42 (i)	DTR C scp42 (ii)	XGB E tai100a (i)	XGB E tai100a (ii)	RFR C tai100a (i)	RFR C tai100a (ii)
nug20.dat	10	393.8	588.3	542.2	1265.7	529.5	4026.2	514.7	1497.0	510.9
nug21.dat	9	495.6	720.5	481.4	963.9	655.2	14835.7	537.3	995.6	645.9
nug22.dat	10	410.2	1517.4	656.0	1594.9	627.4	2766.9	534.4	3125.0	626.2
nug24.dat	10	442.2	4435.4	448.5	1870.7	667.3	1800.7	497.5	2035.6	662.1
nug25.dat	10	667.7	2574.8	700.3	1749.8	965.6	1068.1	665.1	1407.7	951.7
nug27.dat	10	800.8	1233.1	768.1	1767.5	715.9	2018.1	737.9	1523.9	699.7
nug28.dat	9	606.3	986.2	539.9	1319.2	743.4	931.6	568.2	1043.0	727.0
nug30.dat	10	706.5	700.5	587.5	636.9	622.5	965.6	574.1	661.6	597.0
rou12.dat	10	292.3	29546.3	666.2	10189.5	683.3	21386.0	586.8	8453.3	400.2
rou15.dat	10	519.7	768.4	547.7	2337.8	578.9	6079.0	553.0	6893.5	708.6
rou20.dat	10	587.1	726.7	607.4	1075.3	657.9	769.4	661.5	826.9	675.8
scp41	10	811.5	876.7	585.9	957.9	782.3	771.5	624.9	711.8	661.2
scp410	10	1040.3	1020.7	641.5	648.0	667.1	1240.9	598.7	797.2	687.1
scp42	10	1299.7	676.3	523.2	539.5	595.7	612.1	605.2	651.2	639.1
scp43	10	1779.7	576.6	529.7	620.3	495.7	1047.9	710.8	660.1	657.3
scp44	10	1173.6	829.4	591.5	601.4	570.7	894.2	630.2	696.1	705.7
scp45	10	1386.6	607.6	531.6	369.0	699.1	818.6	625.8	673.3	654.4
scp46	10	1359.3	953.5	569.7	608.9	589.8	919.2	574.6	614.8	646.5
scp47	10	1252.6	800.7	594.3	450.8	461.3	2346.1	587.2	617.5	473.1
scp48	10	930.8	659.5	662.9	344.6	704.6	769.3	599.1	709.8	712.2
scp49	10	1011.4	736.8	612.6	1090.5	734.5	823.6	618.7	883.2	837.2
scp51	10	1172.8	737.7	696.3	524.1	783.3	992.3	672.2	830.7	825.3
scp510	10	925.6	734.3	415.1	737.0	593.8	663.4	427.4	668.8	660.3
scp52	10	994.0	641.4	404.2	723.8	656.6	641.0	430.9	608.5	570.1
scp53	10	1322.8	1018.7	488.6	492.5	552.6	956.3	554.4	627.0	530.5
scp54	10	1028.0	950.6	540.4	543.2	734.8	726.0	558.2	636.5	627.1
scp55	10	1233.7	599.4	455.6	1212.2	742.2	1159.3	603.4	558.6	499.6
scp56	10	1248.3	1627.8	669.2	610.1	645.2	814.1	670.7	956.9	768.5
scp57	10	927.4	711.0	620.5	910.3	844.3	1003.9	619.7	803.3	694.8
scp58	10	987.1	707.3	554.9	766.7	642.3	656.4	550.0	721.5	736.9
scp59	10	1132.1	1181.5	696.4	940.8	812.4	936.3	769.5	780.3	762.0
scp61	10	1671.4	966.3	695.3	690.6	588.6	853.0	667.9	732.0	661.2
scp62	10	1332.8	603.7	513.8	683.8	559.0	1007.8	578.4	524.5	525.5
scp63	10	2522.9	816.3	576.3	805.2	737.5	1101.2	547.0	830.2	758.4
scp64	10	2843.9	3516.1	524.2	885.9	432.7	910.1	522.9	841.0	444.3
scp65	9	2010.8	510.1	523.6	618.7	516.9	840.5	539.1	553.0	539.2
scpa1	10	939.5	593.9	469.1	556.6	605.4	889.4	599.5	664.6	566.3

Instance	Num. (Execs.)	Prob. Stop (i)	XGB E scp42 (i)	XGB E scp42 (ii)	DTR C scp42 (i)	DTR C scp42 (ii)	XGB E tai100a (i)	XGB E tai100a (ii)	RFR C tai100a (i)	RFR C tai100a (ii)
scpa2	10	671.8	717.5	467.3	857.5	551.0	855.1	440.3	492.6	523.4
scpa3	10	784.9	509.7	485.5	541.9	493.4	642.8	471.8	713.2	694.3
scpa4	10	954.5	695.2	523.6	312.0	480.7	760.7	567.4	598.2	607.0
scpa5	10	826.8	928.7	610.9	684.0	628.7	1054.2	682.0	713.9	717.0
scpb1	10	3107.6	516.0	446.1	560.0	481.0	619.9	416.6	463.0	450.5
scpb2	10	3859.9	743.3	539.2	562.4	587.3	798.7	524.1	602.9	562.6
scpb3	10	3560.8	963.2	572.7	710.9	646.4	935.7	637.1	705.8	635.8
scpb4	10	3511.4	996.6	573.3	793.4	711.9	1032.1	524.5	705.7	692.7
scpb5	10	3593.9	880.2	726.4	788.6	771.9	1016.4	781.5	740.1	753.0
scpc1	10	644.5	701.6	387.8	631.4	450.2	628.5	503.4	508.8	522.7
scpc2	10	862.6	677.8	576.5	584.8	522.0	650.3	563.7	716.8	681.6
scpc3	10	656.7	562.8	408.1	453.5	401.4	905.8	427.7	591.3	543.2
scpc4	10	840.0	735.2	526.7	454.8	470.6	666.5	579.7	675.5	663.0
scpc5	10	1086.2	938.5	718.2	639.1	613.7	1267.8	645.5	947.4	868.7
scpd1	10	3267.0	552.6	472.4	582.5	563.5	761.7	504.1	584.6	527.8
scpd2	10	3952.4	732.8	502.9	575.3	619.8	1086.3	644.3	558.2	580.1
scpd3	10	3548.0	846.5	723.6	848.6	872.6	865.7	770.2	832.8	842.0
scpd4	10	3491.1	486.7	456.6	617.0	662.4	705.4	511.6	586.0	618.5
scpd5	10	3098.8	1045.2	572.6	783.1	693.3	866.0	531.0	740.4	670.4
scr12.dat	10	374.4	661.5	661.3	14039.0	635.6	95656.6	594.7	20011.5	630.9
scr15.dat	10	656.4	1237.9	468.3	6145.7	616.6	4910.4	523.8	6496.2	585.9
scr20.dat	10	429.3	918.7	396.2	949.2	446.4	1303.4	600.7	813.9	417.9
sko100a.dat	10	4104.4	757.2	529.4	1643.3	465.1	4534.4	535.9	1196.1	536.4
sko100b.dat	10	505.8	3526.8	532.1	1280.2	496.5	718.6	436.0	768.8	600.5
sko100c.dat	9	289.4	719.7	441.7	638.5	473.6	511.7	495.2	619.0	625.3
sko100d.dat	10	779.2	823.7	465.1	663.0	512.9	773.2	668.8	587.3	571.7
sko100e.dat	10	884.7	672.3	652.0	804.9	586.6	988.8	575.1	724.5	626.7
sko100f.dat	10	503.7	747.0	492.0	700.3	441.0	617.9	545.0	545.0	481.9
sko42.dat	10	843.4	719.8	516.7	658.3	450.8	845.6	478.4	523.2	490.5
sko49.dat	10	883.2	738.7	595.9	842.0	703.3	730.2	620.6	837.6	826.4
sko56.dat	10	1164.0	1331.0	596.3	657.9	629.4	920.5	591.5	722.3	642.1
sko64.dat	10	1041.3	1429.2	640.4	867.6	720.9	1304.0	600.7	725.8	681.4
sko72.dat	10	930.1	894.2	682.1	939.9	771.7	853.0	764.6	909.3	908.5
sko81.dat	10	742.1	787.0	567.2	794.9	634.1	781.2	554.5	754.9	743.2
sko90.dat	10	1006.9	740.0	533.1	838.0	619.4	1034.5	538.2	726.1	671.1
ste36a.dat	10	790.0	665.4	497.0	614.6	626.6	994.6	559.2	609.2	596.2
ste36b.dat	10	986.7	569.1	405.7	509.0	526.8	640.4	497.0	511.5	495.4

Instance	Num. (Execs.)	Prob. Stop (i)	XGB E scp42 (i)	XGB E scp42 (ii)	DTR C scp42 (i)	DTR C scp42 (ii)	XGB E tai100a (i)	XGB E tai100a (ii)	RFR C tai100a (i)	RFR C tai100a (ii)
ste36c.dat	10	1231.7	685.8	720.4	635.7	644.8	897.7	699.3	616.9	621.6
tai100a.dat	8	1231.4	2976.5	609.5	3929.1	527.2	12069.3	596.7	836.0	530.5
tai100b.dat	4	2363.1	489.7	420.5	551.5	564.8	796.4	452.6	577.6	551.4
tai12a.dat	10	521.9	39922.2	610.4	44260.8	695.9	18346.5	661.5	17390.0	610.3
tai12b.dat	10	441.7	1517.8	452.3	4855.7	605.7	3883.1	593.4	4188.7	569.9
tai15a.dat	10	483.0	1999.1	458.9	1850.5	589.0	1399.0	591.0	1652.3	568.5
tai15b.dat	10	468.5	21109.9	581.0	5208.1	626.0	19864.9	476.1	9519.5	620.1
tai17a.dat	10	606.0	1396.0	448.5	1286.2	718.2	1124.8	550.7	899.1	471.3
tai20a.dat	10	395.4	681.3	403.6	719.7	669.8	587.7	442.7	552.7	490.4
tai20b.dat	10	449.6	4477.5	599.0	2631.6	769.1	773.9	507.5	2645.7	737.3
tai25a.dat	10	632.1	758.3	601.8	442.3	672.3	738.6	594.5	911.9	767.3
tai25b.dat	10	490.1	1422.8	558.2	1304.0	699.0	1589.2	677.2	1309.8	673.5
tai30a.dat	10	548.8	686.6	468.7	848.3	614.9	763.5	559.1	744.5	722.8
tai30b.dat	10	515.7	845.3	546.1	759.0	788.3	1398.7	543.2	786.6	759.3
tai35a.dat	7	471.5	938.1	451.0	3050.8	510.9	952.3	452.2	643.9	468.7
tai35b.dat	10	25310.2	815.9	603.0	725.4	735.5	710.4	534.7	750.6	722.6
tai40a.dat	10	877.7	1183.6	610.2	1533.2	628.9	1004.1	693.1	778.6	747.5
tai40b.dat	10	6525.2	997.6	537.3	640.1	573.8	666.2	673.1	674.9	551.8
tai50a.dat	10	791.3	847.8	672.4	1623.7	650.4	657.6	628.9	902.5	753.6
tai50b.dat	10	12129.5	736.7	552.2	480.9	474.5	1159.7	480.8	518.9	458.2
tai60a.dat	10	517.3	502.8	562.3	1202.5	579.8	1066.1	459.8	554.6	558.3
tai60b.dat	10	13905.9	886.0	650.4	944.4	940.3	733.0	660.7	909.5	917.3
tai64c.dat	9	299.8	6557.6	762.9	25252.6	508.9	34952.7	618.2	21767.9	504.6
tai80a.dat	10	819.0	1203.6	694.4	1540.9	742.1	944.7	631.9	936.0	826.3
tai80b.dat	10	786.6	895.4	502.8	567.8	596.6	634.9	442.5	535.4	561.3
tho30.dat	10	908.4	663.5	493.2	1090.9	675.7	1510.9	617.6	897.8	655.5
tho40.dat	10	598.2	806.6	498.8	624.1	641.5	581.2	399.2	624.8	613.2
wil100.dat	10	871.7	873.9	702.3	858.7	896.7	872.9	749.1	875.2	860.9
wil50.dat	10	1569.9	685.8	571.8	623.5	614.6	685.8	536.0	595.9	587.7

Appendix C

Stopping Rule in Action

Instance	Model	Num. of Executions	Avg. Time ML Stop (s)	Avg. Time Prob. Stop (s)	Avg. Num. of Estimator Runs
bur26d.dat	DTR_C_scp42	10	0.0069	1749.288	7
bur26d.dat	XGB_E_scp42	10	0.0528	1749.288	7
chr22a.dat	DTR_C_scp42	10	0.0054	1608.485	12
chr22a.dat	XGB_E_scp42	10	0.0295	1608.485	12
esc16j.dat	DTR_C_scp42	10	0.0066	1845.561	1
esc16j.dat	XGB_E_scp42	10	0.0491	1845.561	1
had12.dat	DTR_C_scp42	10	0.0050	1350.334	3
had12.dat	XGB_E_scp42	10	0.0239	1350.334	3
lipa20a.dat	DTR_C_scp42	10	0.0051	1494.675	5
lipa20a.dat	XGB_E_scp42	10	0.0256	1494.675	5
nug12.dat	DTR_C_scp42	10	0.0055	1533.873	4
nug12.dat	XGB_E_scp42	10	0.0310	1533.873	4
rou20.dat	DTR_C_scp42	10	0.0051	1436.249	8
rou20.dat	XGB_E_scp42	10	0.0291	1436.249	8
scp410	DTR_C_scp42	10	0.0154	1.469	18014
scp410	XGB_E_scp42	10	0.1722	1.469	18014
scp42	DTR_C_scp42	10	0.0126	1.303	20014
scp42	XGB_E_scp42	10	0.2187	1.303	20014
scp49	DTR_C_scp42	10	0.0156	1.469	20014
scp49	XGB_E_scp42	10	0.1990	1.469	20014
scp51	DTR_C_scp42	10	0.0187	1.984	20014
scp51	XGB_E_scp42	10	0.0737	1.984	20014
scp65	DTR_C_scp42	10	0.0110	1.272	20014
scp65	XGB_E_scp42	10	0.1808	1.272	20014
scpa4	DTR_C_scp42	10	0.0084	1.290	20012
scpa4	XGB_E_scp42	10	0.0751	1.290	20012
scpb3	DTR_C_scp42	10	0.0084	1.129	20012
scpb3	XGB_E_scp42	10	0.0746	1.129	20012
scpc1	DTR_C_scp42	10	0.0070	1.049	20012
scpc1	XGB_E_scp42	10	0.0503	1.049	20012
scpd1	DTR_C_scp42	10	0.0085	1.250	20013
scpd1	XGB_E_scp42	10	0.0623	1.250	20013
scpd5	DTR_C_scp42	10	0.0070	1.073	20015
scpd5	XGB_E_scp42	10	0.0442	1.073	20015
sko56.dat	DTR_C_scp42	10	0.0047	1355.716	15
sko56.dat	XGB_E_scp42	10	0.0218	1355.716	15
tai30a.dat	DTR_C_scp42	10	0.0047	1356.414	16
tai30a.dat	XGB_E_scp42	10	0.0236	1356.414	16
wil50.dat	DTR_C_scp42	10	0.0046	1399.951	15
wil50.dat	XGB_E_scp42	10	0.0232	1399.951	15

Table C.1: Aggregate results for estimation time. Feature sets are from Table 3.6.

Table C.2: Comparison between the ML-based and the CDF-based stopping rules on 20 different instances (10 QAP and 10 SCP). Feature set codes come from Table 3.6.

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
bur26d	11568	DTR C scp42	0.100000	2	0.038658	0.232689	2	0.044535	0.232689
			0.010000	41	0.000041	0.007913	41	0.002976	0.007913
			0.001000	41	0.000041	0.007913	60	0.000541	0.002746
			0.000100	41	0.000041	0.007913	229	0.000000	0.000000
			0.000010	—	—	—	229	0.000000	0.000000
			0.000001	—	—	—	229	0.000000	0.000000
bur26d	11568	XGB E scp42	0.100000	25	0.007959	0.058678	2	0.044535	0.232689
			0.010000	25	0.007959	0.058678	41	0.002976	0.007913
			0.001000	—	—	—	60	0.000541	0.002746
			0.000100	—	—	—	229	0.000000	0.000000
			0.000010	—	—	—	229	0.000000	0.000000
			0.000001	—	—	—	229	0.000000	0.000000
bur26d	25959	DTR C scp42	0.100000	2	0.038658	0.385607	6	0.064114	0.255767
			0.010000	6	0.000722	0.255767	10	0.006528	0.058014
			0.001000	6	0.000722	0.255767	373	0.000248	0.001011
			0.000100	49	0.000041	0.012976	490	0.000000	0.000000
			0.000010	—	—	—	490	0.000000	0.000000
			0.000001	—	—	—	490	0.000000	0.000000
bur26d	25959	XGB E scp42	0.100000	6	0.080365	0.255767	6	0.064114	0.255767
			0.010000	17	0.000647	0.017570	10	0.006528	0.058014
			0.001000	17	0.000647	0.017570	373	0.000248	0.001011
			0.000100	—	—	—	490	0.000000	0.000000
			0.000010	—	—	—	490	0.000000	0.000000
			0.000001	—	—	—	490	0.000000	0.000000
bur26d	26843	DTR C scp42	0.100000	2	0.038658	0.425234	9	0.019214	0.199338
			0.010000	6	0.000722	0.365817	23	0.003895	0.017738
			0.001000	6	0.000722	0.365817	158	0.000000	0.000000
			0.000100	—	—	—	158	0.000000	0.000000
			0.000010	—	—	—	158	0.000000	0.000000
			0.000001	—	—	—	158	0.000000	0.000000
bur26d	26843	XGB E scp42	0.100000	9	0.055233	0.199338	9	0.019214	0.199338
			0.010000	21	0.003686	0.178959	23	0.003895	0.017738
			0.001000	—	—	—	158	0.000000	0.000000
			0.000100	—	—	—	158	0.000000	0.000000
			0.000010	—	—	—	158	0.000000	0.000000
			0.000001	—	—	—	158	0.000000	0.000000
bur26d	28707	DTR C scp42	0.100000	2	0.038658	0.540705	3	0.047008	0.246648
			0.010000	15	0.000615	0.017512	15	0.006703	0.017512
			0.001000	15	0.000615	0.017512	423	0.000529	0.002353
			0.000100	—	—	—	667	0.000000	0.000000
			0.000010	—	—	—	667	0.000000	0.000000
			0.000001	—	—	—	667	0.000000	0.000000
bur26d	28707	XGB E scp42	0.100000	15	0.007507	0.017512	3	0.047008	0.246648
			0.010000	15	0.007507	0.017512	15	0.006703	0.017512
			0.001000	—	—	—	423	0.000529	0.002353
			0.000100	—	—	—	667	0.000000	0.000000
			0.000010	—	—	—	667	0.000000	0.000000
			0.000001	—	—	—	667	0.000000	0.000000
bur26d	30860	DTR C scp42	0.100000	2	0.038658	0.050146	2	0.049539	0.050146
			0.010000	7	0.000722	0.001435	7	0.000366	0.001435
			0.001000	7	0.000722	0.001435	7	0.000366	0.001435
			0.000100	—	—	—	1200	0.000000	0.000000
			0.000010	—	—	—	1200	0.000000	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	1200	0.000000	0.000000
bur26d	30860	XGB E scp42	0.100000	7	0.093716	0.001435	2	0.049539	0.050146
			0.010000	1200	0.000080	0.000000	7	0.000366	0.001435
			0.001000	1200	0.000080	0.000000	7	0.000366	0.001435
			0.000100	1200	0.000080	0.000000	1200	0.000000	0.000000
			0.000010	—	—	—	1200	0.000000	0.000000
			0.000001	—	—	—	1200	0.000000	0.000000
bur26d	34016	DTR C scp42	0.100000	2	0.038658	0.090076	2	0.041623	0.090076
			0.010000	5	0.000722	0.049603	17	0.005189	0.017592
			0.001000	5	0.000722	0.049603	719	0.000224	0.000629
			0.000100	46	0.000041	0.006722	948	0.000000	0.000000
			0.000010	—	—	—	948	0.000000	0.000000
			0.000001	—	—	—	948	0.000000	0.000000
bur26d	34016	XGB E scp42	0.100000	17	0.021248	0.017592	2	0.041623	0.090076
			0.010000	458	0.000506	0.004154	17	0.005189	0.017592
			0.001000	458	0.000506	0.004154	719	0.000224	0.000629
			0.000100	—	—	—	948	0.000000	0.000000
			0.000010	—	—	—	948	0.000000	0.000000
			0.000001	—	—	—	948	0.000000	0.000000
bur26d	43984	DTR C scp42	0.100000	2	0.038658	0.156559	2	0.076668	0.156559
			0.010000	7	0.000722	0.017568	7	0.009169	0.017568
			0.001000	7	0.000722	0.017568	430	0.000000	0.000000
			0.000100	—	—	—	430	0.000000	0.000000
			0.000010	—	—	—	430	0.000000	0.000000
			0.000001	—	—	—	430	0.000000	0.000000
bur26d	43984	XGB E scp42	0.100000	7	0.073106	0.017568	2	0.076668	0.156559
			0.010000	125	0.005754	0.009959	7	0.009169	0.017568
			0.001000	—	—	—	430	0.000000	0.000000
			0.000100	—	—	—	430	0.000000	0.000000
			0.000010	—	—	—	430	0.000000	0.000000
			0.000001	—	—	—	430	0.000000	0.000000
bur26d	56384	DTR C scp42	0.100000	2	0.038658	0.310904	3	0.034111	0.185812
			0.010000	5	0.000722	0.061150	28	0.006610	0.039244
			0.001000	5	0.000722	0.061150	205	0.000235	0.001142
			0.000100	42	0.000041	0.017643	1574	0.000000	0.000000
			0.000010	—	—	—	1574	0.000000	0.000000
			0.000001	—	—	—	1574	0.000000	0.000000
bur26d	56384	XGB E scp42	0.100000	5	0.073736	0.061150	3	0.034111	0.185812
			0.010000	42	0.006718	0.017643	28	0.006610	0.039244
			0.001000	1574	0.000367	0.000000	205	0.000235	0.001142
			0.000100	—	—	—	1574	0.000000	0.000000
			0.000010	—	—	—	1574	0.000000	0.000000
			0.000001	—	—	—	1574	0.000000	0.000000
bur26d	82394	DTR C scp42	0.100000	2	0.038658	0.351795	10	0.028584	0.229050
			0.010000	5	0.000722	0.281350	78	0.003926	0.012891
			0.001000	5	0.000722	0.281350	157	0.000506	0.002707
			0.000100	—	—	—	184	0.000000	0.000000
			0.000010	—	—	—	184	0.000000	0.000000
			0.000001	—	—	—	184	0.000000	0.000000
bur26d	82394	XGB E scp42	0.100000	5	0.071295	0.281350	10	0.028584	0.229050
			0.010000	19	0.002256	0.055228	78	0.003926	0.012891
			0.001000	—	—	—	157	0.000506	0.002707
			0.000100	—	—	—	184	0.000000	0.000000
			0.000010	—	—	—	184	0.000000	0.000000
			0.000001	—	—	—	184	0.000000	0.000000
bur26d	86397	DTR C scp42	0.100000	2	0.038658	0.110277	2	0.053864	0.110277
			0.010000	38	0.000136	0.017529	38	0.005822	0.017529

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	38	0.000136	0.017529	93	0.000537	0.002637
			0.000100	—	—	—	375	0.000000	0.000000
			0.000010	—	—	—	375	0.000000	0.000000
			0.000001	—	—	—	375	0.000000	0.000000
bur26d	86397	XGB E scp42	0.100000	38	0.024862	0.017529	2	0.053864	0.110277
			0.010000	93	0.008951	0.002637	38	0.005822	0.017529
			0.001000	—	—	—	93	0.000537	0.002637
			0.000100	—	—	—	375	0.000000	0.000000
			0.000010	—	—	—	375	0.000000	0.000000
			0.000001	—	—	—	375	0.000000	0.000000
chr22a	29215	DTR C scp42	0.100000	2	0.038658	0.432166	14	0.016564	0.047345
			0.010000	7	0.000722	0.283793	460	0.009164	0.004806
			0.001000	7	0.000722	0.283793	4126	0.000289	0.000000
			0.000100	66502	0.000019	0.000000	177609	0.000080	0.000000
			0.000010	177609	0.000005	0.000000	575565	0.000000	0.000000
			0.000001	575565	0.000001	0.000000	575565	0.000000	0.000000
chr22a	29215	XGB E scp42	0.100000	7	0.073106	0.283793	14	0.016564	0.047345
			0.010000	16	0.000131	0.013722	460	0.009164	0.004806
			0.001000	16	0.000131	0.013722	4126	0.000289	0.000000
			0.000100	66502	0.000017	0.000000	177609	0.000080	0.000000
			0.000010	177609	0.000003	0.000000	575565	0.000000	0.000000
			0.000001	575565	0.000001	0.000000	575565	0.000000	0.000000
chr22a	36899	DTR C scp42	0.100000	2	0.038658	0.013036	168	0.008168	0.010281
			0.010000	168	0.001554	0.010281	168	0.008168	0.010281
			0.001000	1541	0.000578	0.000000	5810	0.000000	0.000000
			0.000100	—	—	—	5810	0.000000	0.000000
			0.000010	—	—	—	5810	0.000000	0.000000
			0.000001	—	—	—	5810	0.000000	0.000000
chr22a	36899	XGB E scp42	0.100000	168	0.009524	0.010281	168	0.008168	0.010281
			0.010000	168	0.009524	0.010281	168	0.008168	0.010281
			0.001000	1541	0.000547	0.000000	5810	0.000000	0.000000
			0.000100	—	—	—	5810	0.000000	0.000000
			0.000010	—	—	—	5810	0.000000	0.000000
			0.000001	—	—	—	5810	0.000000	0.000000
chr22a	39706	DTR C scp42	0.100000	2	0.038658	0.315186	4	0.066918	0.046262
			0.010000	8	0.000722	0.000221	14296	0.000687	0.000000
			0.001000	8	0.000722	0.000221	14296	0.000687	0.000000
			0.000100	14296	0.000069	0.000000	695732	0.000000	0.000000
			0.000010	100507	0.000007	0.000000	695732	0.000000	0.000000
			0.000001	695732	0.000000	0.000000	695732	0.000000	0.000000
chr22a	39706	XGB E scp42	0.100000	4	0.093594	0.046262	4	0.066918	0.046262
			0.010000	14296	0.000051	0.000000	14296	0.000687	0.000000
			0.001000	14296	0.000051	0.000000	14296	0.000687	0.000000
			0.000100	14296	0.000051	0.000000	695732	0.000000	0.000000
			0.000010	100507	0.000008	0.000000	695732	0.000000	0.000000
			0.000001	695732	0.000000	0.000000	695732	0.000000	0.000000
chr22a	48860	DTR C scp42	0.100000	2	0.038658	0.467080	8	0.060960	0.375610
			0.010000	8	0.000722	0.375610	119	0.006920	0.001349
			0.001000	8	0.000722	0.375610	15734	0.000687	0.000000
			0.000100	15734	0.000069	0.000000	381338	0.000081	0.000000
			0.000010	183895	0.000002	0.000000	830239	0.000000	0.000000
			0.000001	381338	0.000001	0.000000	830239	0.000000	0.000000
chr22a	48860	XGB E scp42	0.100000	8	0.086416	0.375610	8	0.060960	0.375610
			0.010000	13	-0.003411	0.021421	119	0.006920	0.001349
			0.001000	13	-0.003411	0.021421	15734	0.000687	0.000000
			0.000100	13	-0.003411	0.021421	381338	0.000081	0.000000
			0.000010	13	-0.003411	0.021421	830239	0.000000	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	13	-0.003411	0.021421	830239	0.000000	0.000000
chr22a	49783	DTR C scp42	0.100000	2	0.038658	0.267930	4	0.092048	0.066218
			0.010000	10	0.000722	0.016058	35	0.006928	0.010216
			0.001000	10	0.000722	0.016058	18661	0.000471	0.000000
			0.000100	49	0.000041	0.002515	441661	0.000000	0.000000
			0.000010	441661	0.000001	0.000000	441661	0.000000	0.000000
			0.000001	441661	0.000001	0.000000	441661	0.000000	0.000000
chr22a	49783	XGB E scp42	0.100000	4	0.093594	0.066218	4	0.092048	0.066218
			0.010000	35	0.007252	0.010216	35	0.006928	0.010216
			0.001000	910	0.000471	0.000000	18661	0.000471	0.000000
			0.000100	5481	0.000069	0.000000	441661	0.000000	0.000000
			0.000010	14428	0.000001	0.000000	441661	0.000000	0.000000
			0.000001	14428	0.000001	0.000000	441661	0.000000	0.000000
chr22a	57027	DTR C scp42	0.100000	2	0.038658	0.153912	13	0.039919	0.084765
			0.010000	13	0.000615	0.084765	105	0.008416	0.003219
			0.001000	13	0.000615	0.084765	3368	0.000744	0.000000
			0.000100	53	0.000041	0.006915	112537	0.000000	0.000000
			0.000010	87694	0.000007	0.000000	112537	0.000000	0.000000
			0.000001	—	—	—	112537	0.000000	0.000000
chr22a	57027	XGB E scp42	0.100000	13	0.032767	0.084765	13	0.039919	0.084765
			0.010000	105	0.007815	0.003219	105	0.008416	0.003219
			0.001000	1104	0.000607	0.000000	3368	0.000744	0.000000
			0.000100	23371	0.000044	0.000000	112537	0.000000	0.000000
			0.000010	87694	0.000009	0.000000	112537	0.000000	0.000000
			0.000001	—	—	—	112537	0.000000	0.000000
chr22a	59775	DTR C scp42	0.100000	2	0.038658	0.093197	7	0.053734	0.059178
			0.010000	7	0.000722	0.059178	167	0.006463	0.001237
			0.001000	7	0.000722	0.059178	42033	0.000480	0.000000
			0.000100	35883	0.000028	0.000000	174626	0.000000	0.000000
			0.000010	103053	0.000007	0.000000	174626	0.000000	0.000000
			0.000001	—	—	—	174626	0.000000	0.000000
chr22a	59775	XGB E scp42	0.100000	7	0.093716	0.059178	7	0.053734	0.059178
			0.010000	92	0.008189	0.004764	167	0.006463	0.001237
			0.001000	1998	0.000476	0.000000	42033	0.000480	0.000000
			0.000100	35883	0.000041	0.000000	174626	0.000000	0.000000
			0.000010	103053	0.000004	0.000000	174626	0.000000	0.000000
			0.000001	—	—	—	174626	0.000000	0.000000
chr22a	75756	DTR C scp42	0.100000	2	0.038658	0.154703	6	0.074583	0.078699
			0.010000	6	0.000722	0.078699	1879	0.005540	0.000000
			0.001000	6	0.000722	0.078699	18416	0.000671	0.000000
			0.000100	55	0.000041	0.007511	59355	0.000087	0.000000
			0.000010	306856	0.000002	0.000000	306856	0.000000	0.000000
			0.000001	—	—	—	306856	0.000000	0.000000
chr22a	75756	XGB E scp42	0.100000	6	0.077613	0.078699	6	0.074583	0.078699
			0.010000	1879	0.000464	0.000000	1879	0.005540	0.000000
			0.001000	1879	0.000464	0.000000	18416	0.000671	0.000000
			0.000100	13793	0.000041	0.000000	59355	0.000087	0.000000
			0.000010	306856	0.000002	0.000000	306856	0.000000	0.000000
			0.000001	—	—	—	306856	0.000000	0.000000
chr22a	95393	DTR C scp42	0.100000	2	0.038658	0.931355	4	0.053578	0.865666
			0.010000	5	0.000722	0.505098	48	0.004491	0.000068
			0.001000	5	0.000722	0.505098	6529	0.000622	0.000000
			0.000100	48	0.000041	0.000068	53527	0.000084	0.000000
			0.000010	—	—	—	61060	0.000000	0.000000
			0.000001	—	—	—	61060	0.000000	0.000000
chr22a	95393	XGB E scp42	0.100000	4	0.093594	0.865666	4	0.053578	0.865666
			0.010000	17	0.001041	0.004126	48	0.004491	0.000068

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	6529	0.000020	0.000000	6529	0.000622	0.000000
			0.000100	6529	0.000020	0.000000	53527	0.000084	0.000000
			0.000010	—	—	—	61060	0.000000	0.000000
			0.000001	—	—	—	61060	0.000000	0.000000
chr22a	99105	DTR C scp42	0.100000	2	0.038658	0.033695	53	0.015956	0.009349
			0.010000	53	0.000041	0.009349	119	0.008171	0.001346
			0.001000	53	0.000041	0.009349	52205	0.000476	0.000000
			0.000100	53	0.000041	0.009349	256597	0.000080	0.000000
			0.000010	124370	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
chr22a	99105	XGB E scp42	0.100000	53	0.017188	0.009349	53	0.015956	0.009349
			0.010000	119	0.009057	0.001346	119	0.008171	0.001346
			0.001000	5989	0.000143	0.000000	52205	0.000476	0.000000
			0.000100	6325	0.000030	0.000000	256597	0.000080	0.000000
			0.000010	7290	0.000008	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	12486	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	12486	XGB E scp42	0.100000	2	0.000000	0.000000	2	0.001210	0.000000
			0.010000	2	0.000000	0.000000	2	0.001210	0.000000
			0.001000	2	0.000000	0.000000	—	—	—
			0.000100	2	0.000000	0.000000	—	—	—
			0.000010	2	0.000000	0.000000	—	—	—
			0.000001	2	0.000000	0.000000	—	—	—
esc16j	17729	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	17729	XGB E scp42	0.100000	—	—	—	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	19630	DTR C scp42	0.100000	2	0.038658	0.529186	4	0.000772	0.000000
			0.010000	—	—	—	4	0.000772	0.000000
			0.001000	—	—	—	4	0.000772	0.000000
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	19630	XGB E scp42	0.100000	4	0.092657	0.000000	4	0.000772	0.000000
			0.010000	—	—	—	4	0.000772	0.000000
			0.001000	—	—	—	4	0.000772	0.000000
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	29762	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—

Instance	Seed	Model	β	**Iteration (ML S.)**	**Probs. (ML S.)**	**Expected (ML S.)**	**Iteration (Prob. S.)**	**Probs. (Prob. S.)**	**Expected (Prob. S.)**
			0.000001	—	—	—	—	—	—
esc16j	29762	XGB E scp42	0.100000	2	0.000000	0.000000	2	0.002420	0.000000
			0.010000	2	0.000000	0.000000	2	0.002420	0.000000
			0.001000	2	0.000000	0.000000	—	—	—
			0.000100	2	0.000000	0.000000	—	—	—
			0.000010	2	0.000000	0.000000	—	—	—
			0.000001	2	0.000000	0.000000	—	—	—
esc16j	38873	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	38873	XGB E scp42	0.100000	2	0.000000	0.000000	2	0.002420	0.000000
			0.010000	2	0.000000	0.000000	2	0.002420	0.000000
			0.001000	2	0.000000	0.000000	—	—	—
			0.000100	2	0.000000	0.000000	—	—	—
			0.000010	2	0.000000	0.000000	—	—	—
			0.000001	2	0.000000	0.000000	—	—	—
esc16j	5804	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	5804	XGB E scp42	0.100000	—	—	—	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	75601	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	75601	XGB E scp42	0.100000	—	—	—	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	84287	DTR C scp42	0.100000	2	0.038658	0.528455	4	0.001038	0.000000
			0.010000	—	—	—	4	0.001038	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	84287	XGB E scp42	0.100000	2	0.000000	0.528455	4	0.001038	0.000000
			0.010000	2	0.000000	0.528455	4	0.001038	0.000000
			0.001000	2	0.000000	0.528455	—	—	—
			0.000100	2	0.000000	0.528455	—	—	—
			0.000010	2	0.000000	0.528455	—	—	—
			0.000001	2	0.000000	0.528455	—	—	—
esc16j	88062	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	88062	XGB E scp42	0.100000	—	—	—	2	0.001210	0.000000
			0.010000	—	—	—	2	0.001210	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	93071	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
esc16j	93071	XGB E scp42	0.100000	—	—	—	2	0.002420	0.000000
			0.010000	—	—	—	2	0.002420	0.000000
			0.001000	—	—	—	—	—	—
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	10946	DTR C scp42	0.100000	2	0.064610	0.494329	14	0.030672	0.087722
			0.010000	14	0.000615	0.087722	27	0.000029	0.000000
			0.001000	14	0.000615	0.087722	27	0.000029	0.000000
			0.000100	—	—	—	27	0.000029	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	10946	XGB E scp42	0.100000	14	0.015966	0.087722	14	0.030672	0.087722
			0.010000	—	—	—	27	0.000029	0.000000
			0.001000	—	—	—	27	0.000029	0.000000
			0.000100	—	—	—	27	0.000029	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	20183	DTR C scp42	0.100000	2	0.038658	0.228375	9	0.036952	0.088450
			0.010000	9	0.000722	0.088450	112	0.000033	0.000000
			0.001000	9	0.000722	0.088450	112	0.000033	0.000000
			0.000100	—	—	—	112	0.000033	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	20183	XGB E scp42	0.100000	9	0.037635	0.088450	9	0.036952	0.088450
			0.010000	112	0.009036	0.000000	112	0.000033	0.000000
			0.001000	—	—	—	112	0.000033	0.000000
			0.000100	—	—	—	112	0.000033	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	20856	DTR C scp42	0.100000	2	0.038658	0.088234	19	0.021668	0.031933
			0.010000	19	0.003334	0.031933	55	0.000067	0.000000
			0.001000	44	0.000041	0.018999	55	0.000067	0.000000
			0.000100	44	0.000041	0.018999	55	0.000067	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	20856	XGB E scp42	0.100000	19	0.021223	0.031933	19	0.021668	0.031933
			0.010000	—	—	—	55	0.000067	0.000000
			0.001000	—	—	—	55	0.000067	0.000000
			0.000100	—	—	—	55	0.000067	0.000000
			0.000010	—	—	—	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
had12	23994	DTR C scp42	0.100000	2	0.082691	0.088957	2	0.072534	0.088957
			0.010000	46	0.000041	0.000000	46	0.000064	0.000000
			0.001000	46	0.000041	0.000000	46	0.000064	0.000000
			0.000100	46	0.000041	0.000000	46	0.000064	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	23994	XGB E scp42	0.100000	22	0.011795	0.019285	2	0.072534	0.088957
			0.010000	—	—	—	46	0.000064	0.000000
			0.001000	—	—	—	46	0.000064	0.000000
			0.000100	—	—	—	46	0.000064	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	31185	DTR C scp42	0.100000	2	0.038658	0.263348	4	0.000097	0.000000
			0.010000	—	—	—	4	0.000097	0.000000
			0.001000	—	—	—	4	0.000097	0.000000
			0.000100	—	—	—	4	0.000097	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	31185	XGB E scp42	0.100000	—	—	—	4	0.000097	0.000000
			0.010000	—	—	—	4	0.000097	0.000000
			0.001000	—	—	—	4	0.000097	0.000000
			0.000100	—	—	—	4	0.000097	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	58640	DTR C scp42	0.100000	2	0.038658	0.422168	6	0.023495	0.228191
			0.010000	6	0.000722	0.228191	18	0.000076	0.000000
			0.001000	6	0.000722	0.228191	18	0.000076	0.000000
			0.000100	—	—	—	18	0.000076	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	58640	XGB E scp42	0.100000	6	0.096174	0.228191	6	0.023495	0.228191
			0.010000	—	—	—	18	0.000076	0.000000
			0.001000	—	—	—	18	0.000076	0.000000
			0.000100	—	—	—	18	0.000076	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	65186	DTR C scp42	0.100000	2	0.038658	0.000000	2	0.000173	0.000000
			0.010000	—	—	—	2	0.000173	0.000000
			0.001000	—	—	—	2	0.000173	0.000000
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	65186	XGB E scp42	0.100000	—	—	—	2	0.000173	0.000000
			0.010000	—	—	—	2	0.000173	0.000000
			0.001000	—	—	—	2	0.000173	0.000000
			0.000100	—	—	—	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	68019	DTR C scp42	0.100000	2	0.038658	0.228780	7	0.048350	0.088188
			0.010000	7	0.000722	0.088188	62	0.000054	0.000000
			0.001000	7	0.000722	0.088188	62	0.000054	0.000000
			0.000100	—	—	—	62	0.000054	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	68019	XGB E scp42	0.100000	7	0.091220	0.088188	7	0.048350	0.088188
			0.010000	—	—	—	62	0.000054	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	—	—	—	62	0.000054	0.000000
			0.000100	—	—	—	62	0.000054	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	71640	DTR C scp42	0.100000	2	0.038658	0.550155	3	0.019587	0.018788
			0.010000	47	0.000041	0.000000	47	0.000057	0.000000
			0.001000	47	0.000041	0.000000	47	0.000057	0.000000
			0.000100	47	0.000041	0.000000	47	0.000057	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	71640	XGB E scp42	0.100000	47	0.026680	0.000000	3	0.019587	0.018788
			0.010000	—	—	—	47	0.000057	0.000000
			0.001000	—	—	—	47	0.000057	0.000000
			0.000100	—	—	—	47	0.000057	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	89516	DTR C scp42	0.100000	2	0.038658	0.550108	3	0.063179	0.088387
			0.010000	11	0.000722	0.031767	15	0.000079	0.000000
			0.001000	11	0.000722	0.031767	15	0.000079	0.000000
			0.000100	—	—	—	15	0.000079	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
had12	89516	XGB E scp42	0.100000	11	0.035486	0.031767	3	0.063179	0.088387
			0.010000	15	0.003926	0.000000	15	0.000079	0.000000
			0.001000	—	—	—	15	0.000079	0.000000
			0.000100	—	—	—	15	0.000079	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
lipa20a	31658	DTR C scp42	0.100000	11	0.076644	0.143486	5	0.032251	0.268661
			0.010000	83	0.006300	0.000000	44	0.005265	0.030605
			0.001000	—	—	—	83	0.000000	0.000000
			0.000100	—	—	—	83	0.000000	0.000000
			0.000010	—	—	—	83	0.000000	0.000000
			0.000001	—	—	—	83	0.000000	0.000000
lipa20a	31658	XGB E scp42	0.100000	5	0.068412	0.268661	5	0.032251	0.268661
			0.010000	11	0.006314	0.143486	44	0.005265	0.030605
			0.001000	13	0.000457	0.080923	83	0.000000	0.000000
			0.000100	—	—	—	83	0.000000	0.000000
			0.000010	—	—	—	83	0.000000	0.000000
			0.000001	—	—	—	83	0.000000	0.000000
lipa20a	56829	DTR C scp42	0.100000	2	0.064610	0.047477	34	0.020181	0.039269
			0.010000	175	0.001554	0.007140	55	0.000662	0.016904
			0.001000	—	—	—	55	0.000662	0.016904
			0.000100	—	—	—	175	0.000000	0.007140
			0.000010	—	—	—	175	0.000000	0.007140
			0.000001	—	—	—	175	0.000000	0.007140
lipa20a	56829	XGB E scp42	0.100000	2	0.000000	0.047477	34	0.020181	0.039269
			0.010000	2	0.000000	0.047477	55	0.000662	0.016904
			0.001000	2	0.000000	0.047477	55	0.000662	0.016904
			0.000100	2	0.000000	0.047477	175	0.000000	0.007140
			0.000010	2	0.000000	0.047477	175	0.000000	0.007140
			0.000001	2	0.000000	0.047477	175	0.000000	0.007140
lipa20a	63372	DTR C scp42	0.100000	4	0.093271	0.143630	8	0.072519	0.047077
			0.010000	33	0.002215	0.011275	33	0.000129	0.011275
			0.001000	—	—	—	33	0.000129	0.011275
			0.000100	—	—	—	74	0.000003	0.006752
			0.000010	—	—	—	74	0.000003	0.006752

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	343	0.000000	0.000000
lipa20a	63372	XGB E scp42	0.100000	4	0.091413	0.143630	8	0.072519	0.047077
			0.010000	33	0.006872	0.011275	33	0.000129	0.011275
			0.001000	—	—	—	33	0.000129	0.011275
			0.000100	—	—	—	74	0.000003	0.006752
			0.000010	—	—	—	74	0.000003	0.006752
			0.000001	—	—	—	343	0.000000	0.000000
lipa20a	65809	DTR C scp42	0.100000	16	0.041762	0.178195	16	0.076967	0.178195
			0.010000	18	0.003334	0.013062	18	0.001008	0.013062
			0.001000	255	0.000259	0.000000	255	0.000000	0.000000
			0.000100	—	—	—	255	0.000000	0.000000
			0.000010	—	—	—	255	0.000000	0.000000
			0.000001	—	—	—	255	0.000000	0.000000
lipa20a	65809	XGB E scp42	0.100000	4	0.092657	0.352283	16	0.076967	0.178195
			0.010000	16	0.000191	0.178195	18	0.001008	0.013062
			0.001000	16	0.000191	0.178195	255	0.000000	0.000000
			0.000100	—	—	—	255	0.000000	0.000000
			0.000010	—	—	—	255	0.000000	0.000000
			0.000001	—	—	—	255	0.000000	0.000000
lipa20a	69991	DTR C scp42	0.100000	6	0.079678	0.101983	3	0.079429	0.295304
			0.010000	74	0.006300	0.010504	74	0.000007	0.010504
			0.001000	232	0.000259	0.000000	74	0.000007	0.010504
			0.000100	—	—	—	74	0.000007	0.010504
			0.000010	—	—	—	74	0.000007	0.010504
			0.000001	—	—	—	232	0.000000	0.000000
lipa20a	69991	XGB E scp42	0.100000	6	0.058785	0.101983	3	0.079429	0.295304
			0.010000	232	0.001699	0.000000	74	0.000007	0.010504
			0.001000	—	—	—	74	0.000007	0.010504
			0.000100	—	—	—	74	0.000007	0.010504
			0.000010	—	—	—	74	0.000007	0.010504
			0.000001	—	—	—	232	0.000000	0.000000
lipa20a	71991	DTR C scp42	0.100000	9	0.013186	0.020336	9	0.013196	0.020336
			0.010000	32	0.002215	0.011985	32	0.000560	0.011985
			0.001000	33	0.000136	0.009547	32	0.000560	0.011985
			0.000100	—	—	—	129	0.000013	0.008696
			0.000010	—	—	—	320	0.000000	0.000000
			0.000001	—	—	—	320	0.000000	0.000000
lipa20a	71991	XGB E scp42	0.100000	9	0.052615	0.020336	9	0.013196	0.020336
			0.010000	33	0.007252	0.009547	32	0.000560	0.011985
			0.001000	—	—	—	32	0.000560	0.011985
			0.000100	—	—	—	129	0.000013	0.008696
			0.000010	—	—	—	320	0.000000	0.000000
			0.000001	—	—	—	320	0.000000	0.000000
lipa20a	74870	DTR C scp42	0.100000	2	0.064610	0.080703	32	0.005440	0.022102
			0.010000	133	0.004777	0.000000	32	0.005440	0.022102
			0.001000	—	—	—	133	0.000000	0.000000
			0.000100	—	—	—	133	0.000000	0.000000
			0.000010	—	—	—	133	0.000000	0.000000
			0.000001	—	—	—	133	0.000000	0.000000
lipa20a	74870	XGB E scp42	0.100000	32	0.024964	0.022102	32	0.005440	0.022102
			0.010000	133	0.005096	0.000000	32	0.005440	0.022102
			0.001000	—	—	—	133	0.000000	0.000000
			0.000100	—	—	—	133	0.000000	0.000000
			0.000010	—	—	—	133	0.000000	0.000000
			0.000001	—	—	—	133	0.000000	0.000000
lipa20a	77357	DTR C scp42	0.100000	6	0.000722	0.005255	6	0.013284	0.005255
			0.010000	6	0.000722	0.005255	12	0.000005	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	6	0.000722	0.005255	12	0.000005	0.000000
			0.000100	—	—	—	12	0.000005	0.000000
			0.000010	—	—	—	12	0.000005	0.000000
			0.000001	—	—	—	—	—	—
lipa20a	77357	XGB E scp42	0.100000	6	0.080769	0.005255	6	0.013284	0.005255
			0.010000	—	—	—	12	0.000005	0.000000
			0.001000	—	—	—	12	0.000005	0.000000
			0.000100	—	—	—	12	0.000005	0.000000
			0.000010	—	—	—	12	0.000005	0.000000
			0.000001	—	—	—	—	—	—
lipa20a	78452	DTR C scp42	0.100000	2	0.082691	0.052343	42	0.004759	0.024228
			0.010000	69	0.006300	0.007225	42	0.004759	0.024228
			0.001000	—	—	—	69	0.000001	0.007225
			0.000100	—	—	—	69	0.000001	0.007225
			0.000010	—	—	—	69	0.000001	0.007225
			0.000001	—	—	—	69	0.000001	0.007225
lipa20a	78452	XGB E scp42	0.100000	42	0.019720	0.024228	42	0.004759	0.024228
			0.010000	187	0.001630	0.000000	42	0.004759	0.024228
			0.001000	—	—	—	69	0.000001	0.007225
			0.000100	—	—	—	69	0.000001	0.007225
			0.000010	—	—	—	69	0.000001	0.007225
			0.000001	—	—	—	69	0.000001	0.007225
lipa20a	9510	DTR C scp42	0.100000	8	0.034460	0.030675	8	0.023964	0.030675
			0.010000	101	0.007058	0.010531	101	0.000001	0.010531
			0.001000	—	—	—	101	0.000001	0.010531
			0.000100	—	—	—	101	0.000001	0.010531
			0.000010	—	—	—	101	0.000001	0.010531
			0.000001	—	—	—	101	0.000001	0.010531
lipa20a	9510	XGB E scp42	0.100000	8	0.082560	0.030675	8	0.023964	0.030675
			0.010000	101	0.008720	0.010531	101	0.000001	0.010531
			0.001000	—	—	—	101	0.000001	0.010531
			0.000100	—	—	—	101	0.000001	0.010531
			0.000010	—	—	—	101	0.000001	0.010531
			0.000001	—	—	—	101	0.000001	0.010531
nug12	23805	DTR C scp42	0.100000	2	0.082691	0.238754	4	0.079092	0.064452
			0.010000	13	0.000615	0.021814	86	0.000027	0.000000
			0.001000	13	0.000615	0.021814	86	0.000027	0.000000
			0.000100	—	—	—	86	0.000027	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	23805	XGB E scp42	0.100000	13	0.081641	0.021814	4	0.079092	0.064452
			0.010000	—	—	—	86	0.000027	0.000000
			0.001000	—	—	—	86	0.000027	0.000000
			0.000100	—	—	—	86	0.000027	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	32751	DTR C scp42	0.100000	2	0.093271	0.744364	3	0.080238	0.459897
			0.010000	6	0.000722	0.154781	21	0.000037	0.000000
			0.001000	6	0.000722	0.154781	21	0.000037	0.000000
			0.000100	—	—	—	21	0.000037	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	32751	XGB E scp42	0.100000	6	0.080043	0.154781	3	0.080238	0.459897
			0.010000	15	0.007322	0.021875	21	0.000037	0.000000
			0.001000	—	—	—	21	0.000037	0.000000
			0.000100	—	—	—	21	0.000037	0.000000
			0.000010	—	—	—	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
nug12	36813	DTR C scp42	0.100000	2	0.064610	0.660896	3	0.080237	0.377932
			0.010000	15	0.000615	0.064475	47	0.000028	0.000000
			0.001000	15	0.000615	0.064475	47	0.000028	0.000000
			0.000100	43	0.000041	0.022042	47	0.000028	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	36813	XGB E scp42	0.100000	15	0.014747	0.064475	3	0.080237	0.377932
			0.010000	47	0.004647	0.000000	47	0.000028	0.000000
			0.001000	—	—	—	47	0.000028	0.000000
			0.000100	—	—	—	47	0.000028	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	55465	DTR C scp42	0.100000	2	0.038658	0.064447	6	0.077421	0.021903
			0.010000	6	0.000722	0.021903	295	0.000041	0.000000
			0.001000	6	0.000722	0.021903	295	0.000041	0.000000
			0.000100	—	—	—	295	0.000041	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	55465	XGB E scp42	0.100000	6	0.078322	0.021903	6	0.077421	0.021903
			0.010000	295	0.001720	0.000000	295	0.000041	0.000000
			0.001000	—	—	—	295	0.000041	0.000000
			0.000100	—	—	—	295	0.000041	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	56813	DTR C scp42	0.100000	2	0.038658	0.341953	5	0.080758	0.064538
			0.010000	5	0.000722	0.064538	25	0.000039	0.000000
			0.001000	5	0.000722	0.064538	25	0.000039	0.000000
			0.000100	—	—	—	25	0.000039	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	56813	XGB E scp42	0.100000	5	0.072493	0.064538	5	0.080758	0.064538
			0.010000	25	0.007972	0.000000	25	0.000039	0.000000
			0.001000	—	—	—	25	0.000039	0.000000
			0.000100	—	—	—	25	0.000039	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	81762	DTR C scp42	0.100000	2	0.093271	0.459122	7	0.043020	0.064047
			0.010000	7	0.000722	0.064047	18	0.000032	0.000000
			0.001000	7	0.000722	0.064047	18	0.000032	0.000000
			0.000100	—	—	—	18	0.000032	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	81762	XGB E scp42	0.100000	4	0.085121	0.238504	7	0.043020	0.064047
			0.010000	18	0.002287	0.000000	18	0.000032	0.000000
			0.001000	—	—	—	18	0.000032	0.000000
			0.000100	—	—	—	18	0.000032	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	84788	DTR C scp42	0.100000	2	0.038658	0.499838	16	0.015234	0.010465
			0.010000	5	0.000722	0.115772	31	0.000045	0.000000
			0.001000	5	0.000722	0.115772	31	0.000045	0.000000
			0.000100	—	—	—	31	0.000045	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	84788	XGB E scp42	0.100000	4	0.091413	0.238967	16	0.015234	0.010465
			0.010000	16	0.000154	0.010465	31	0.000045	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	16	0.000154	0.010465	31	0.000045	0.000000
			0.000100	—	—	—	31	0.000045	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	84858	DTR C scp42	0.100000	2	0.093271	0.021862	2	0.081259	0.021862
			0.010000	5	0.000722	0.010397	41	0.000026	0.000000
			0.001000	5	0.000722	0.010397	41	0.000026	0.000000
			0.000100	41	0.000041	0.000000	41	0.000026	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	84858	XGB E scp42	0.100000	41	0.024327	0.000000	2	0.081259	0.021862
			0.010000	—	—	—	41	0.000026	0.000000
			0.001000	—	—	—	41	0.000026	0.000000
			0.000100	—	—	—	41	0.000026	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	87339	DTR C scp42	0.100000	2	0.038658	0.214440	12	0.047173	0.064076
			0.010000	12	0.000722	0.064076	309	0.000027	0.000000
			0.001000	12	0.000722	0.064076	309	0.000027	0.000000
			0.000100	45	0.000041	0.021760	309	0.000027	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	87339	XGB E scp42	0.100000	12	0.075326	0.064076	12	0.047173	0.064076
			0.010000	309	0.000930	0.000000	309	0.000027	0.000000
			0.001000	309	0.000930	0.000000	309	0.000027	0.000000
			0.000100	—	—	—	309	0.000027	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	97034	DTR C scp42	0.100000	2	0.082691	0.116444	12	0.058219	0.022001
			0.010000	12	0.000722	0.022001	185	0.000030	0.000000
			0.001000	12	0.000722	0.022001	185	0.000030	0.000000
			0.000100	—	—	—	185	0.000030	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
nug12	97034	XGB E scp42	0.100000	12	0.032007	0.022001	12	0.058219	0.022001
			0.010000	185	0.001717	0.000000	185	0.000030	0.000000
			0.001000	—	—	—	185	0.000030	0.000000
			0.000100	—	—	—	185	0.000030	0.000000
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
rou20	34405	DTR C scp42	0.100000	2	0.064610	0.174227	7	0.077401	0.077993
			0.010000	13	0.000615	0.023751	149	0.005467	0.003596
			0.001000	13	0.000615	0.023751	1758	0.000843	0.000000
			0.000100	—	—	—	4322	0.000000	0.000000
			0.000010	—	—	—	4322	0.000000	0.000000
			0.000001	—	—	—	4322	0.000000	0.000000
rou20	34405	XGB E scp42	0.100000	7	0.071467	0.077993	7	0.077401	0.077993
			0.010000	149	0.006095	0.003596	149	0.005467	0.003596
			0.001000	784	0.000463	0.002115	1758	0.000843	0.000000
			0.000100	—	—	—	4322	0.000000	0.000000
			0.000010	—	—	—	4322	0.000000	0.000000
			0.000001	—	—	—	4322	0.000000	0.000000
rou20	35493	DTR C scp42	0.100000	2	0.038658	0.090112	11	0.048024	0.023496
			0.010000	11	0.000722	0.023496	391	0.000039	0.000000
			0.001000	11	0.000722	0.023496	391	0.000039	0.000000
			0.000100	12901	0.000085	0.000000	391	0.000039	0.000000
			0.000010	—	—	—	12901	0.000000	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	12901	0.000000	0.000000
rou20	35493	XGB E scp42	0.100000	11	0.073878	0.023496	11	0.048024	0.023496
			0.010000	90	0.009875	0.012769	391	0.000039	0.000000
			0.001000	12901	0.000017	0.000000	391	0.000039	0.000000
			0.000100	12901	0.000017	0.000000	391	0.000039	0.000000
			0.000010	—	—	—	12901	0.000000	0.000000
			0.000001	—	—	—	12901	0.000000	0.000000
rou20	39000	DTR C scp42	0.100000	2	0.064610	0.121365	9	0.082843	0.087353
			0.010000	12	0.000722	0.010059	177	0.007660	0.009534
			0.001000	12	0.000722	0.010059	1910	0.000020	0.000000
			0.000100	50076	0.000021	0.000000	1910	0.000020	0.000000
			0.000010	—	—	—	50076	0.000000	0.000000
			0.000001	—	—	—	50076	0.000000	0.000000
rou20	39000	XGB E scp42	0.100000	6	0.098222	0.111814	9	0.082843	0.087353
			0.010000	177	0.001891	0.009534	177	0.007660	0.009534
			0.001000	268	0.000648	0.001044	1910	0.000020	0.000000
			0.000100	50076	0.000017	0.000000	1910	0.000020	0.000000
			0.000010	—	—	—	50076	0.000000	0.000000
			0.000001	—	—	—	50076	0.000000	0.000000
rou20	48528	DTR C scp42	0.100000	2	0.082691	0.199654	8	0.012931	0.004459
			0.010000	8	0.000722	0.004459	48	0.003654	0.003072
			0.001000	8	0.000722	0.004459	1576	0.000617	0.000000
			0.000100	48	0.000041	0.003072	23562	0.000000	0.000000
			0.000010	—	—	—	23562	0.000000	0.000000
			0.000001	—	—	—	23562	0.000000	0.000000
rou20	48528	XGB E scp42	0.100000	8	0.081046	0.004459	8	0.012931	0.004459
			0.010000	481	0.000567	0.002101	48	0.003654	0.003072
			0.001000	481	0.000567	0.002101	1576	0.000617	0.000000
			0.000100	9190	0.000003	0.000000	23562	0.000000	0.000000
			0.000010	9190	0.000003	0.000000	23562	0.000000	0.000000
			0.000001	—	—	—	23562	0.000000	0.000000
rou20	54106	DTR C scp42	0.100000	7	0.007752	0.059805	7	0.043209	0.059805
			0.010000	7	0.007752	0.059805	101	0.001077	0.001824
			0.001000	2240	0.000348	0.000000	434	0.000485	0.000264
			0.000100	—	—	—	3672	0.000000	0.000000
			0.000010	—	—	—	3672	0.000000	0.000000
			0.000001	—	—	—	3672	0.000000	0.000000
rou20	54106	XGB E scp42	0.100000	7	0.091220	0.059805	7	0.043209	0.059805
			0.010000	23	0.005731	0.018629	101	0.001077	0.001824
			0.001000	434	0.000657	0.000264	434	0.000485	0.000264
			0.000100	—	—	—	3672	0.000000	0.000000
			0.000010	—	—	—	3672	0.000000	0.000000
			0.000001	—	—	—	3672	0.000000	0.000000
rou20	68699	DTR C scp42	0.100000	2	0.038658	0.046729	46	0.035826	0.036828
			0.010000	46	0.003290	0.036828	385	0.002167	0.002099
			0.001000	757	0.000811	0.000000	757	0.000701	0.000000
			0.000100	—	—	—	2078	0.000000	0.000000
			0.000010	—	—	—	2078	0.000000	0.000000
			0.000001	—	—	—	2078	0.000000	0.000000
rou20	68699	XGB E scp42	0.100000	46	0.025275	0.036828	46	0.035826	0.036828
			0.010000	307	0.001584	0.015236	385	0.002167	0.002099
			0.001000	385	0.000958	0.002099	757	0.000701	0.000000
			0.000100	—	—	—	2078	0.000000	0.000000
			0.000010	—	—	—	2078	0.000000	0.000000
			0.000001	—	—	—	2078	0.000000	0.000000
rou20	81250	DTR C scp42	0.100000	8	0.025506	0.090992	8	0.037704	0.090992
			0.010000	43	0.000041	0.009806	463	0.004444	0.003683

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	43	0.000041	0.009806	1299	0.000377	0.000000
			0.000100	43	0.000041	0.009806	8538	0.000035	0.000000
			0.000010	—	—	—	29820	0.000000	0.000000
			0.000001	—	—	—	29820	0.000000	0.000000
rou20	81250	XGB E scp42	0.100000	8	0.081046	0.090992	8	0.037704	0.090992
			0.010000	43	0.005401	0.009806	463	0.004444	0.003683
			0.001000	1299	0.000470	0.000000	1299	0.000377	0.000000
			0.000100	8538	0.000050	0.000000	8538	0.000035	0.000000
			0.000010	—	—	—	29820	0.000000	0.000000
			0.000001	—	—	—	29820	0.000000	0.000000
rou20	86528	DTR C scp42	0.100000	3	0.082691	0.185738	3	0.087729	0.185738
			0.010000	304	0.001568	0.000000	23	0.008522	0.002561
			0.001000	—	—	—	304	0.000000	0.000000
			0.000100	—	—	—	304	0.000000	0.000000
			0.000010	—	—	—	304	0.000000	0.000000
			0.000001	—	—	—	304	0.000000	0.000000
rou20	86528	XGB E scp42	0.100000	4	0.093703	0.006668	3	0.087729	0.185738
			0.010000	23	0.005731	0.002561	23	0.008522	0.002561
			0.001000	—	—	—	304	0.000000	0.000000
			0.000100	—	—	—	304	0.000000	0.000000
			0.000010	—	—	—	304	0.000000	0.000000
			0.000001	—	—	—	304	0.000000	0.000000
rou20	88406	DTR C scp42	0.100000	2	0.082691	0.259306	12	0.070989	0.193330
			0.010000	70	0.006300	0.001586	70	0.003724	0.001586
			0.001000	5933	0.000180	0.000000	5933	0.000454	0.000000
			0.000100	16175	0.000069	0.000000	7496	0.000015	0.000000
			0.000010	—	—	—	16175	0.000000	0.000000
			0.000001	—	—	—	16175	0.000000	0.000000
rou20	88406	XGB E scp42	0.100000	12	0.026894	0.193330	12	0.070989	0.193330
			0.010000	332	0.000896	0.000425	70	0.003724	0.001586
			0.001000	332	0.000896	0.000425	5933	0.000454	0.000000
			0.000100	5933	0.000034	0.000000	7496	0.000015	0.000000
			0.000010	7496	0.000006	0.000000	16175	0.000000	0.000000
			0.000001	—	—	—	16175	0.000000	0.000000
rou20	95732	DTR C scp42	0.100000	2	0.064610	0.354794	4	0.035796	0.004197
			0.010000	218	0.001554	0.000128	218	0.000245	0.000128
			0.001000	7312	0.000151	0.000000	218	0.000245	0.000128
			0.000100	23265	0.000035	0.000000	7312	0.000015	0.000000
			0.000010	—	—	—	23265	0.000000	0.000000
			0.000001	—	—	—	23265	0.000000	0.000000
rou20	95732	XGB E scp42	0.100000	218	0.010267	0.000128	4	0.035796	0.004197
			0.010000	7312	0.000096	0.000000	218	0.000245	0.000128
			0.001000	7312	0.000096	0.000000	218	0.000245	0.000128
			0.000100	7312	0.000096	0.000000	7312	0.000015	0.000000
			0.000010	—	—	—	23265	0.000000	0.000000
			0.000001	—	—	—	23265	0.000000	0.000000
scp410	16716	DTR C scp42	0.100000	6	0.025506	0.007182	6	0.070552	0.007182
			0.010000	154	0.001554	0.000000	154	0.002112	0.000000
			0.001000	83248	0.000011	0.000000	108559	0.000967	0.000000
			0.000100	83248	0.000011	0.000000	—	—	—
			0.000010	108559	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp410	16716	XGB E scp42	0.100000	6	0.098222	0.007182	6	0.070552	0.007182
			0.010000	83248	0.000005	0.000000	154	0.002112	0.000000
			0.001000	83248	0.000005	0.000000	108559	0.000967	0.000000
			0.000100	83248	0.000005	0.000000	—	—	—
			0.000010	83248	0.000005	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
scp410	20269	DTR C scp42	0.100000	14	0.054826	0.086311	14	0.074967	0.086311
			0.010000	357	0.001120	0.000546	357	0.006568	0.000546
			0.001000	1136	0.000682	0.000000	114094	0.000687	0.000000
			0.000100	72280	0.000013	0.000000	—	—	—
			0.000010	114094	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp410	20269	XGB E scp42	0.100000	14	0.012236	0.086311	14	0.074967	0.086311
			0.010000	41	0.005489	0.002825	357	0.006568	0.000546
			0.001000	357	0.000953	0.000546	114094	0.000687	0.000000
			0.000100	72280	0.000016	0.000000	—	—	—
			0.000010	74618	0.000009	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp410	21246	DTR C scp42	0.100000	4	0.038658	0.015743	23	0.034804	0.011008
			0.010000	109	0.007058	0.004658	222	0.005252	0.000158
			0.001000	151	0.000398	0.001512	31530	0.000806	0.000000
			0.000100	10995	0.000085	0.000000	—	—	—
			0.000010	100525	0.000007	0.000000	—	—	—
			0.000001	344715	0.000001	0.000000	—	—	—
scp410	21246	XGB E scp42	0.100000	23	0.013640	0.011008	23	0.034804	0.011008
			0.010000	109	0.008720	0.004658	222	0.005252	0.000158
			0.001000	3652	0.000433	0.000000	31530	0.000806	0.000000
			0.000100	10995	0.000014	0.000000	—	—	—
			0.000010	100525	0.000004	0.000000	—	—	—
			0.000001	344715	0.000001	0.000000	—	—	—
scp410	39837	DTR C scp42	0.100000	3	0.076681	0.354478	5	0.078386	0.078912
			0.010000	90	0.009318	0.016491	397	0.009439	0.002237
			0.001000	8662	0.000122	0.000000	39768	0.000673	0.000000
			0.000100	21584	0.000035	0.000000	—	—	—
			0.000010	146308	0.000005	0.000000	—	—	—
			0.000001	535922	0.000001	0.000000	—	—	—
scp410	39837	XGB E scp42	0.100000	6	0.079251	0.056143	5	0.078386	0.078912
			0.010000	166	0.005836	0.003136	397	0.009439	0.002237
			0.001000	8662	0.000060	0.000000	39768	0.000673	0.000000
			0.000100	8662	0.000060	0.000000	—	—	—
			0.000010	146308	0.000005	0.000000	—	—	—
			0.000001	535922	0.000001	0.000000	—	—	—
scp410	40055	DTR C scp42	0.100000	22	0.027368	0.015483	7	0.060554	0.085806
			0.010000	42	0.002215	0.000676	93	0.009637	0.000476
			0.001000	704	0.000811	0.000000	39551	0.000576	0.000000
			0.000100	27060	0.000028	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp410	40055	XGB E scp42	0.100000	7	0.071467	0.085806	7	0.060554	0.085806
			0.010000	22	0.003531	0.015483	93	0.009637	0.000476
			0.001000	704	0.000517	0.000000	39551	0.000576	0.000000
			0.000100	5912	0.000077	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp410	4085	DTR C scp42	0.100000	12	0.056393	0.021961	12	0.024688	0.021961
			0.010000	275	0.002501	0.000438	151	0.009581	0.007312
			0.001000	3435	0.000727	0.000000	31568	0.001000	0.000000
			0.000100	31568	0.000028	0.000000	—	—	—
			0.000010	102343	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp410	4085	XGB E scp42	0.100000	5	0.068366	0.365437	12	0.024688	0.021961
			0.010000	161	0.009851	0.004591	151	0.009581	0.007312

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	3435	0.000403	0.000000	31568	0.001000	0.000000
			0.000100	31568	0.000024	0.000000	—	—	—
			0.000010	102343	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp410	45150	DTR C scp42	0.100000	3	0.076681	0.852978	4	0.078983	0.391503
			0.010000	39	0.004795	0.001478	152	0.008536	0.000880
			0.001000	1820	0.000476	0.000000	89264	0.000995	0.000000
			0.000100	19525	0.000056	0.000000	—	—	—
			0.000010	89264	0.000007	0.000000	—	—	—
			0.000001	406554	0.000001	0.000000	—	—	—
scp410	45150	XGB E scp42	0.100000	10	0.070793	0.271419	4	0.078983	0.391503
			0.010000	14	-0.003225	0.003747	152	0.008536	0.000880
			0.001000	14	-0.003225	0.003747	89264	0.000995	0.000000
			0.000100	14	-0.003225	0.003747	—	—	—
			0.000010	14	-0.003225	0.003747	—	—	—
			0.000001	14	-0.003225	0.003747	—	—	—
scp410	5202	DTR C scp42	0.100000	14	0.016479	0.076699	14	0.026542	0.076699
			0.010000	89	0.006300	0.002591	633	0.004660	0.000000
			0.001000	178	0.000398	0.001654	146157	0.000880	0.000000
			0.000100	15816	0.000069	0.000000	—	—	—
			0.000010	146157	0.000005	0.000000	—	—	—
			0.000001	396744	0.000001	0.000000	—	—	—
scp410	5202	XGB E scp42	0.100000	6	0.077613	0.334827	14	0.026542	0.076699
			0.010000	15	0.003926	0.005061	633	0.004660	0.000000
			0.001000	6581	0.000127	0.000000	146157	0.000880	0.000000
			0.000100	15816	0.000077	0.000000	—	—	—
			0.000010	146157	0.000004	0.000000	—	—	—
			0.000001	396744	0.000001	0.000000	—	—	—
scp410	7057	DTR C scp42	0.100000	4	0.064610	0.373790	38	0.015040	0.019485
			0.010000	103	0.007058	0.017974	150	0.004888	0.001473
			0.001000	1403	0.000636	0.000000	87262	0.000497	0.000000
			0.000100	16031	0.000069	0.000000	—	—	—
			0.000010	87262	0.000007	0.000000	—	—	—
			0.000001	404572	0.000001	0.000000	—	—	—
scp410	7057	XGB E scp42	0.100000	4	0.083425	0.373790	38	0.015040	0.019485
			0.010000	13	-0.002281	0.148697	150	0.004888	0.001473
			0.001000	13	-0.002281	0.148697	87262	0.000497	0.000000
			0.000100	13	-0.002281	0.148697	—	—	—
			0.000010	13	-0.002281	0.148697	—	—	—
			0.000001	13	-0.002281	0.148697	—	—	—
scp410	93146	DTR C scp42	0.100000	4	0.054172	0.688495	6	0.088469	0.257091
			0.010000	103	0.007058	0.002461	890	0.005308	0.000000
			0.001000	890	0.000682	0.000000	54154	0.000577	0.000000
			0.000100	15470	0.000069	0.000000	—	—	—
			0.000010	883090	0.000000	0.000000	—	—	—
			0.000001	883090	0.000000	0.000000	—	—	—
scp410	93146	XGB E scp42	0.100000	4	0.083425	0.688495	6	0.088469	0.257091
			0.010000	15	0.008408	0.013927	890	0.005308	0.000000
			0.001000	890	0.000502	0.000000	54154	0.000577	0.000000
			0.000100	15470	0.000070	0.000000	—	—	—
			0.000010	883090	0.000000	0.000000	—	—	—
			0.000001	883090	0.000000	0.000000	—	—	—
scp42	30736	DTR C scp42	0.100000	3	0.082691	0.131915	14	0.078562	0.059905
			0.010000	112	0.007058	0.008864	776	0.007766	0.000163
			0.001000	745	0.000811	0.004306	351474	0.000836	0.000000
			0.000100	12495	0.000085	0.000000	—	—	—
			0.000010	351474	0.000001	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	351474	0.000001	0.000000	—	—	—
scp42	30736	XGB E scp42	0.100000	14	0.016621	0.059905	14	0.078562	0.059905
			0.010000	112	0.008253	0.008864	776	0.007766	0.000163
			0.001000	745	0.000462	0.004306	351474	0.000836	0.000000
			0.000100	12495	0.000025	0.000000	—	—	—
			0.000010	85150	0.000007	0.000000	—	—	—
			0.000001	351474	0.000001	0.000000	—	—	—
scp42	40849	DTR C scp42	0.100000	3	0.064610	0.231323	4	0.088859	0.073886
			0.010000	273	0.002501	0.012760	1767	0.005270	0.000000
			0.001000	345	0.000154	0.007653	175303	0.000961	0.000000
			0.000100	87103	0.000007	0.000000	—	—	—
			0.000010	87103	0.000007	0.000000	—	—	—
			0.000001	618700	0.000001	0.000000	—	—	—
scp42	40849	XGB E scp42	0.100000	19	0.020575	0.059564	4	0.088859	0.073886
			0.010000	23	0.005731	0.019547	1767	0.005270	0.000000
			0.001000	1536	0.000376	0.000008	175303	0.000961	0.000000
			0.000100	87103	0.000005	0.000000	—	—	—
			0.000010	87103	0.000005	0.000000	—	—	—
			0.000001	618700	0.000000	0.000000	—	—	—
scp42	41442	DTR C scp42	0.100000	4	0.064610	0.510226	5	0.055927	0.101839
			0.010000	105	0.007058	0.012705	517	0.008360	0.000286
			0.001000	333	0.000154	0.008083	280467	0.000972	0.000000
			0.000100	103806	0.000007	0.000000	—	—	—
			0.000010	103806	0.000007	0.000000	—	—	—
			0.000001	582460	0.000001	0.000000	—	—	—
scp42	41442	XGB E scp42	0.100000	4	0.081438	0.510226	5	0.055927	0.101839
			0.010000	19	0.002435	0.039499	517	0.008360	0.000286
			0.001000	103806	0.000006	0.000000	280467	0.000972	0.000000
			0.000100	103806	0.000006	0.000000	—	—	—
			0.000010	103806	0.000006	0.000000	—	—	—
			0.000001	582460	0.000001	0.000000	—	—	—
scp42	43030	DTR C scp42	0.100000	8	0.032036	0.031257	8	0.053163	0.031257
			0.010000	56	0.004795	0.005784	124	0.004478	0.000114
			0.001000	777	0.000682	0.000000	764585	0.000637	0.000000
			0.000100	19003	0.000056	0.000000	—	—	—
			0.000010	125357	0.000006	0.000000	—	—	—
			0.000001	764585	0.000000	0.000000	—	—	—
scp42	43030	XGB E scp42	0.100000	8	0.037940	0.031257	8	0.053163	0.031257
			0.010000	124	0.005576	0.000114	124	0.004478	0.000114
			0.001000	777	0.000628	0.000000	764585	0.000637	0.000000
			0.000100	19003	0.000090	0.000000	—	—	—
			0.000010	125357	0.000004	0.000000	—	—	—
			0.000001	764585	0.000000	0.000000	—	—	—
scp42	49396	DTR C scp42	0.100000	3	0.038658	0.006636	86	0.017350	0.005669
			0.010000	86	0.006300	0.005669	702	0.008353	0.001334
			0.001000	702	0.000811	0.001334	315964	0.000976	0.000000
			0.000100	17047	0.000064	0.000000	—	—	—
			0.000010	112504	0.000006	0.000000	—	—	—
			0.000001	362265	0.000001	0.000000	—	—	—
scp42	49396	XGB E scp42	0.100000	86	0.010974	0.005669	86	0.017350	0.005669
			0.010000	257	0.003061	0.004161	702	0.008353	0.001334
			0.001000	702	0.000609	0.001334	315964	0.000976	0.000000
			0.000100	5716	0.000060	0.000000	—	—	—
			0.000010	112504	0.000004	0.000000	—	—	—
			0.000001	362265	0.000001	0.000000	—	—	—
scp42	61403	DTR C scp42	0.100000	13	0.094824	0.028893	4	0.081021	0.154227
			0.010000	109	0.007058	0.018901	160	0.006276	0.003257

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	2466	0.000822	0.000000	184698	0.000557	0.000000
			0.000100	9956	0.000078	0.000000	—	—	—
			0.000010	184698	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp42	61403	XGB E scp42	0.100000	7	0.077649	0.115941	4	0.081021	0.154227
			0.010000	109	0.007695	0.018901	160	0.006276	0.003257
			0.001000	2466	0.000319	0.000000	184698	0.000557	0.000000
			0.000100	7427	0.000037	0.000000	—	—	—
			0.000010	15283	0.000001	0.000000	—	—	—
			0.000001	15283	0.000001	0.000000	—	—	—
scp42	67807	DTR C scp42	0.100000	223	0.010204	0.009993	223	0.019076	0.009993
			0.010000	289	0.002501	0.003749	718	0.009745	0.002315
			0.001000	718	0.000811	0.002315	472054	0.000964	0.000000
			0.000100	18994	0.000056	0.000000	—	—	—
			0.000010	207926	0.000002	0.000000	—	—	—
			0.000001	472054	0.000001	0.000000	—	—	—
scp42	67807	XGB E scp42	0.100000	223	0.019961	0.009993	223	0.019076	0.009993
			0.010000	289	0.003897	0.003749	718	0.009745	0.002315
			0.001000	718	0.000597	0.002315	472054	0.000964	0.000000
			0.000100	40066	0.000024	0.000000	—	—	—
			0.000010	207926	0.000002	0.000000	—	—	—
			0.000001	472054	0.000001	0.000000	—	—	—
scp42	72368	DTR C scp42	0.100000	8	0.007752	0.004699	8	0.030394	0.004699
			0.010000	8	0.007752	0.004699	242	0.007826	0.000199
			0.001000	242	0.000259	0.000199	20270	0.000625	0.000000
			0.000100	11010	0.000085	0.000000	—	—	—
			0.000010	531973	0.000001	0.000000	—	—	—
			0.000001	531973	0.000001	0.000000	—	—	—
scp42	72368	XGB E scp42	0.100000	4	0.081438	0.209261	8	0.030394	0.004699
			0.010000	242	0.001690	0.000199	242	0.007826	0.000199
			0.001000	4661	0.000342	0.000000	20270	0.000625	0.000000
			0.000100	9468	0.000033	0.000000	—	—	—
			0.000010	11010	0.000004	0.000000	—	—	—
			0.000001	531973	0.000001	0.000000	—	—	—
scp42	79312	DTR C scp42	0.100000	6	0.071008	0.053568	8	0.099527	0.031082
			0.010000	9	0.007752	0.005523	488	0.008913	0.002068
			0.001000	772	0.000811	0.001306	200670	0.000329	0.000000
			0.000100	52336	0.000021	0.000000	—	—	—
			0.000010	200670	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp42	79312	XGB E scp42	0.100000	6	0.095635	0.053568	8	0.099527	0.031082
			0.010000	220	0.001022	0.004416	488	0.008913	0.002068
			0.001000	488	0.000518	0.002068	200670	0.000329	0.000000
			0.000100	52336	0.000034	0.000000	—	—	—
			0.000010	200670	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp42	82541	DTR C scp42	0.100000	14	0.043227	0.061019	14	0.064691	0.061019
			0.010000	96	0.007058	0.026465	573	0.009947	0.001660
			0.001000	756	0.000811	0.000000	683198	0.000539	0.000000
			0.000100	95074	0.000007	0.000000	—	—	—
			0.000010	95074	0.000007	0.000000	—	—	—
			0.000001	584004	0.000001	0.000000	—	—	—
scp42	82541	XGB E scp42	0.100000	14	0.016621	0.061019	14	0.064691	0.061019
			0.010000	96	0.008442	0.026465	573	0.009947	0.001660
			0.001000	756	0.000492	0.000000	683198	0.000539	0.000000
			0.000100	95074	0.000004	0.000000	—	—	—
			0.000010	95074	0.000004	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	584004	0.000000	0.000000	—	—	—
scp49	32335	DTR C scp42	0.100000	6	0.032036	0.004833	43	0.040462	0.004631
			0.010000	545	0.006412	0.001220	545	0.007624	0.001220
			0.001000	1014	0.000682	0.000000	39020	0.000425	0.000000
			0.000100	10738	0.000085	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp49	32335	XGB E scp42	0.100000	6	0.098222	0.004833	43	0.040462	0.004631
			0.010000	545	0.000120	0.001220	545	0.007624	0.001220
			0.001000	545	0.000120	0.001220	39020	0.000425	0.000000
			0.000100	10738	0.000012	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp49	41076	DTR C scp42	0.100000	14	0.034460	0.026884	4	0.089342	0.289711
			0.010000	138	0.009486	0.012137	166	0.008349	0.000787
			0.001000	1899	0.000476	0.000000	28115	0.000935	0.000000
			0.000100	15227	0.000069	0.000000	—	—	—
			0.000010	131747	0.000005	0.000000	—	—	—
			0.000001	362645	0.000001	0.000000	—	—	—
scp49	41076	XGB E scp42	0.100000	5	0.070941	0.186815	4	0.089342	0.289711
			0.010000	14	0.000442	0.026884	166	0.008349	0.000787
			0.001000	14	0.000442	0.026884	28115	0.000935	0.000000
			0.000100	15227	0.000072	0.000000	—	—	—
			0.000010	131747	0.000005	0.000000	—	—	—
			0.000001	225572	0.000001	0.000000	—	—	—
scp49	41624	DTR C scp42	0.100000	3	0.076681	0.790643	4	0.084348	0.678482
			0.010000	406	0.002333	0.004554	8	0.009047	0.026416
			0.001000	18345	0.000060	0.000000	89592	0.000648	0.000000
			0.000100	18345	0.000060	0.000000	—	—	—
			0.000010	89592	0.000007	0.000000	—	—	—
			0.000001	812580	0.000000	0.000000	—	—	—
scp49	41624	XGB E scp42	0.100000	4	0.092714	0.678482	4	0.084348	0.678482
			0.010000	407	0.003853	0.004396	8	0.009047	0.026416
			0.001000	18345	0.000097	0.000000	89592	0.000648	0.000000
			0.000100	18345	0.000097	0.000000	—	—	—
			0.000010	89592	0.000006	0.000000	—	—	—
			0.000001	812580	0.000000	0.000000	—	—	—
scp49	43633	DTR C scp42	0.100000	18	0.016479	0.058721	18	0.044419	0.058721
			0.010000	311	0.002979	0.003776	54	0.009513	0.012867
			0.001000	920	0.000682	0.000000	5234	0.000652	0.000000
			0.000100	98435	0.000007	0.000000	—	—	—
			0.000010	98435	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp49	43633	XGB E scp42	0.100000	18	0.020929	0.058721	18	0.044419	0.058721
			0.010000	159	0.006217	0.007379	54	0.009513	0.012867
			0.001000	920	0.000458	0.000000	5234	0.000652	0.000000
			0.000100	98435	0.000005	0.000000	—	—	—
			0.000010	98435	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp49	5178	DTR C scp42	0.100000	22	0.027368	0.018814	22	0.027315	0.018814
			0.010000	135	0.004777	0.000097	135	0.004868	0.000097
			0.001000	15611	0.000069	0.000000	128054	0.000524	0.000000
			0.000100	15611	0.000069	0.000000	—	—	—
			0.000010	128054	0.000006	0.000000	—	—	—
			0.000001	361123	0.000001	0.000000	—	—	—
scp49	5178	XGB E scp42	0.100000	7	0.071467	0.206742	22	0.027315	0.018814
			0.010000	53	0.007113	0.004754	135	0.004868	0.000097

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	15611	0.000018	0.000000	128054	0.000524	0.000000
			0.000100	15611	0.000018	0.000000	—	—	—
			0.000010	128054	0.000004	0.000000	—	—	—
			0.000001	361123	0.000001	0.000000	—	—	—
scp49	54948	DTR C scp42	0.100000	14	0.019625	0.100160	14	0.097574	0.100160
			0.010000	139	0.009486	0.024690	156	0.008671	0.003804
			0.001000	1206	0.000636	0.000000	56926	0.000766	0.000000
			0.000100	17742	0.000064	0.000000	—	—	—
			0.000010	514700	0.000001	0.000000	—	—	—
			0.000001	514700	0.000001	0.000000	—	—	—
scp49	54948	XGB E scp42	0.100000	5	0.071295	0.235875	14	0.097574	0.100160
			0.010000	14	-0.002055	0.100160	156	0.008671	0.003804
			0.001000	14	-0.002055	0.100160	56926	0.000766	0.000000
			0.000100	14	-0.002055	0.100160	—	—	—
			0.000010	14	-0.002055	0.100160	—	—	—
			0.000001	14	-0.002055	0.100160	—	—	—
scp49	59035	DTR C scp42	0.100000	33	0.016873	0.002036	4	0.079135	0.295344
			0.010000	917	0.000682	0.000000	33	0.008200	0.002036
			0.001000	917	0.000682	0.000000	106524	0.000984	0.000000
			0.000100	10159	0.000078	0.000000	—	—	—
			0.000010	106524	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp49	59035	XGB E scp42	0.100000	8	0.083620	0.072469	4	0.079135	0.295344
			0.010000	917	0.000571	0.000000	33	0.008200	0.002036
			0.001000	917	0.000571	0.000000	106524	0.000984	0.000000
			0.000100	10159	0.000040	0.000000	—	—	—
			0.000010	106524	0.000008	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp49	75655	DTR C scp42	0.100000	135	0.004777	0.003768	6	0.090484	0.106585
			0.010000	135	0.004777	0.003768	280	0.009449	0.001168
			0.001000	868	0.000682	0.000465	21632	0.000860	0.000000
			0.000100	21632	0.000035	0.000000	—	—	—
			0.000010	370314	0.000001	0.000000	—	—	—
			0.000001	370314	0.000001	0.000000	—	—	—
scp49	75655	XGB E scp42	0.100000	6	0.076935	0.106585	6	0.090484	0.106585
			0.010000	135	0.005086	0.003768	280	0.009449	0.001168
			0.001000	280	0.000731	0.001168	21632	0.000860	0.000000
			0.000100	8456	0.000051	0.000000	—	—	—
			0.000010	79717	0.000007	0.000000	—	—	—
			0.000001	370314	0.000001	0.000000	—	—	—
scp49	85957	DTR C scp42	0.100000	5	0.079678	0.023098	5	0.052434	0.023098
			0.010000	100	0.007058	0.009605	542	0.009053	0.002436
			0.001000	907	0.000682	0.000842	11960	0.000886	0.000000
			0.000100	11960	0.000085	0.000000	—	—	—
			0.000010	86941	0.000007	0.000000	—	—	—
			0.000001	391457	0.000001	0.000000	—	—	—
scp49	85957	XGB E scp42	0.100000	81	0.013197	0.013660	5	0.052434	0.023098
			0.010000	100	0.008940	0.009605	542	0.009053	0.002436
			0.001000	542	0.000504	0.002436	11960	0.000886	0.000000
			0.000100	11960	0.000053	0.000000	—	—	—
			0.000010	86941	0.000005	0.000000	—	—	—
			0.000001	391457	0.000001	0.000000	—	—	—
scp49	91691	DTR C scp42	0.100000	14	0.016479	0.003049	14	0.040243	0.003049
			0.010000	656	0.001233	0.000000	656	0.003012	0.000000
			0.001000	2501	0.000822	0.000000	34815	0.000699	0.000000
			0.000100	11477	0.000085	0.000000	—	—	—
			0.000010	101132	0.000007	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
scp49	91691	XGB E scp42	0.100000	4	0.092714	0.102385	14	0.040243	0.003049
			0.010000	14	-0.002055	0.003049	656	0.003012	0.000000
			0.001000	14	-0.002055	0.003049	34815	0.000699	0.000000
			0.000100	14	-0.002055	0.003049	—	—	—
			0.000010	14	-0.002055	0.003049	—	—	—
			0.000001	14	-0.002055	0.003049	—	—	—
scp51	16627	DTR C scp42	0.100000	5	0.013186	0.008098	5	0.062135	0.008098
			0.010000	70	0.006300	0.001957	70	0.005580	0.001957
			0.001000	4389	0.000266	0.000000	20276	0.000912	0.000000
			0.000100	10423	0.000078	0.000000	—	—	—
			0.000010	112723	0.000006	0.000000	—	—	—
			0.000001	505401	0.000001	0.000000	—	—	—
scp51	16627	XGB E scp42	0.100000	70	0.021450	0.001957	5	0.062135	0.008098
			0.010000	193	0.001510	0.001010	70	0.005580	0.001957
			0.001000	4389	0.000395	0.000000	20276	0.000912	0.000000
			0.000100	8967	0.000027	0.000000	—	—	—
			0.000010	112723	0.000005	0.000000	—	—	—
			0.000001	505401	0.000001	0.000000	—	—	—
scp51	23086	DTR C scp42	0.100000	7	0.056393	0.031090	15	0.070165	0.005621
			0.010000	284	0.000259	0.000568	284	0.007215	0.000568
			0.001000	284	0.000259	0.000568	55325	0.000932	0.000000
			0.000100	15441	0.000069	0.000000	—	—	—
			0.000010	173128	0.000005	0.000000	—	—	—
			0.000001	398061	0.000001	0.000000	—	—	—
scp51	23086	XGB E scp42	0.100000	7	0.077649	0.031090	15	0.070165	0.005621
			0.010000	15	0.007503	0.005621	284	0.007215	0.000568
			0.001000	284	0.000733	0.000568	55325	0.000932	0.000000
			0.000100	15441	0.000041	0.000000	—	—	—
			0.000010	173128	0.000003	0.000000	—	—	—
			0.000001	398061	0.000001	0.000000	—	—	—
scp51	37447	DTR C scp42	0.100000	5	0.079678	0.062219	5	0.059966	0.062219
			0.010000	120	0.007058	0.004330	597	0.007924	0.000205
			0.001000	184	0.000398	0.003639	211654	0.000781	0.000000
			0.000100	13962	0.000069	0.000000	—	—	—
			0.000010	211654	0.000002	0.000000	—	—	—
			0.000001	733792	0.000000	0.000000	—	—	—
scp51	37447	XGB E scp42	0.100000	5	0.070941	0.062219	5	0.059966	0.062219
			0.010000	256	0.005993	0.001352	597	0.007924	0.000205
			0.001000	4557	0.000556	0.000000	211654	0.000781	0.000000
			0.000100	9619	0.000036	0.000000	—	—	—
			0.000010	211654	0.000001	0.000000	—	—	—
			0.000001	211654	0.000001	0.000000	—	—	—
scp51	41845	DTR C scp42	0.100000	3	0.076681	0.487531	6	0.030997	0.008319
			0.010000	80	0.006300	0.000666	80	0.005968	0.000666
			0.001000	1273	0.000636	0.000000	420014	0.000853	0.000000
			0.000100	18735	0.000060	0.000000	—	—	—
			0.000010	420014	0.000001	0.000000	—	—	—
			0.000001	420014	0.000001	0.000000	—	—	—
scp51	41845	XGB E scp42	0.100000	80	0.012515	0.000666	6	0.030997	0.008319
			0.010000	1273	0.000113	0.000000	80	0.005968	0.000666
			0.001000	1273	0.000113	0.000000	420014	0.000853	0.000000
			0.000100	18735	0.000087	0.000000	—	—	—
			0.000010	420014	0.000002	0.000000	—	—	—
			0.000001	646750	0.000000	0.000000	—	—	—
scp51	44929	DTR C scp42	0.100000	8	0.013186	0.009771	8	0.036056	0.009771
			0.010000	509	0.001623	0.004151	2540	0.007827	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	800	0.000682	0.002067	68894	0.000721	0.000000
			0.000100	10176	0.000078	0.000000	—	—	—
			0.000010	328284	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp51	44929	XGB E scp42	0.100000	7	0.077649	0.340866	8	0.036056	0.009771
			0.010000	180	0.001533	0.008614	2540	0.007827	0.000000
			0.001000	509	0.000572	0.004151	68894	0.000721	0.000000
			0.000100	7016	0.000096	0.000000	—	—	—
			0.000010	328284	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp51	51345	DTR C scp42	0.100000	40	0.019047	0.092358	40	0.056778	0.092358
			0.010000	93	0.007058	0.003001	93	0.006511	0.003001
			0.001000	700	0.000811	0.001211	34863	0.000765	0.000000
			0.000100	34863	0.000028	0.000000	—	—	—
			0.000010	145593	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp51	51345	XGB E scp42	0.100000	5	0.072493	0.433968	40	0.056778	0.092358
			0.010000	40	0.007435	0.092358	93	0.006511	0.003001
			0.001000	700	0.000482	0.001211	34863	0.000765	0.000000
			0.000100	4916	0.000064	0.000000	—	—	—
			0.000010	145593	0.000001	0.000000	—	—	—
			0.000001	145593	0.000001	0.000000	—	—	—
scp51	72544	DTR C scp42	0.100000	17	0.054826	0.107152	17	0.073228	0.107152
			0.010000	99	0.007058	0.013281	174	0.008118	0.005371
			0.001000	386	0.000606	0.004705	37263	0.000943	0.000000
			0.000100	16786	0.000064	0.000000	—	—	—
			0.000010	527879	0.000001	0.000000	—	—	—
			0.000001	527879	0.000001	0.000000	—	—	—
scp51	72544	XGB E scp42	0.100000	17	0.021248	0.107152	17	0.073228	0.107152
			0.010000	99	0.009671	0.013281	174	0.008118	0.005371
			0.001000	1227	0.000845	0.000039	37263	0.000943	0.000000
			0.000100	16786	0.000087	0.000000	—	—	—
			0.000010	80823	0.000005	0.000000	—	—	—
			0.000001	527879	0.000001	0.000000	—	—	—
scp51	72556	DTR C scp42	0.100000	3	0.093271	0.060829	70	0.004093	0.002100
			0.010000	70	0.006300	0.002100	70	0.004093	0.002100
			0.001000	1549	0.000578	0.000000	13500	0.000706	0.000000
			0.000100	12213	0.000085	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp51	72556	XGB E scp42	0.100000	7	0.077643	0.047416	70	0.004093	0.002100
			0.010000	500	0.000579	0.001080	70	0.004093	0.002100
			0.001000	500	0.000579	0.001080	13500	0.000706	0.000000
			0.000100	8619	0.000005	0.000000	—	—	—
			0.000010	8619	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp51	75543	DTR C scp42	0.100000	6	0.071008	0.030678	6	0.069291	0.030678
			0.010000	535	0.003038	0.001215	535	0.008558	0.001215
			0.001000	1438	0.000636	0.000000	56629	0.000698	0.000000
			0.000100	30445	0.000028	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp51	75543	XGB E scp42	0.100000	6	0.080188	0.030678	6	0.069291	0.030678
			0.010000	535	0.000553	0.001215	535	0.008558	0.001215
			0.001000	535	0.000553	0.001215	56629	0.000698	0.000000
			0.000100	30445	0.000042	0.000000	—	—	—
			0.000010	—	—	—	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
scp51	93582	DTR C scp42	0.100000	34	0.004795	0.003467	5	0.096031	0.312483
			0.010000	34	0.004795	0.003467	34	0.006522	0.003467
			0.001000	992	0.000682	0.000000	507162	0.000685	0.000000
			0.000100	21114	0.000035	0.000000	—	—	—
			0.000010	121918	0.000006	0.000000	—	—	—
			0.000001	507162	0.000001	0.000000	—	—	—
scp51	93582	XGB E scp42	0.100000	5	0.070941	0.312483	5	0.096031	0.312483
			0.010000	34	0.008257	0.003467	34	0.006522	0.003467
			0.001000	992	0.000482	0.000000	507162	0.000685	0.000000
			0.000100	21114	0.000040	0.000000	—	—	—
			0.000010	121918	0.000005	0.000000	—	—	—
			0.000001	507162	0.000001	0.000000	—	—	—
scp65	15292	DTR C scp42	0.100000	4	0.038658	0.210955	4	0.082148	0.210955
			0.010000	40	0.000136	0.023018	565	0.008586	0.000000
			0.001000	40	0.000136	0.023018	—	—	—
			0.000100	13388	0.000085	0.000000	—	—	—
			0.000010	339022	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	15292	XGB E scp42	0.100000	4	0.094001	0.210955	4	0.082148	0.210955
			0.010000	13	-0.003448	0.133240	565	0.008586	0.000000
			0.001000	13	-0.003448	0.133240	—	—	—
			0.000100	13	-0.003448	0.133240	—	—	—
			0.000010	13	-0.003448	0.133240	—	—	—
			0.000001	13	-0.003448	0.133240	—	—	—
scp65	17913	DTR C scp42	0.100000	3	0.038658	0.093832	10	0.096232	0.056065
			0.010000	10	0.000722	0.056065	2043	0.006743	0.000000
			0.001000	10	0.000722	0.056065	215507	0.000869	0.000000
			0.000100	33764	0.000028	0.000000	—	—	—
			0.000010	134891	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	17913	XGB E scp42	0.100000	10	0.042282	0.056065	10	0.096232	0.056065
			0.010000	275	0.001705	0.001888	2043	0.006743	0.000000
			0.001000	605	0.000519	0.000186	215507	0.000869	0.000000
			0.000100	5846	0.000054	0.000000	—	—	—
			0.000010	77634	0.000008	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	23847	DTR C scp42	0.100000	3	0.054172	0.431519	4	0.095596	0.038341
			0.010000	44	0.000041	0.025659	361	0.009244	0.000035
			0.001000	44	0.000041	0.025659	—	—	—
			0.000100	44	0.000041	0.025659	—	—	—
			0.000010	167458	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	23847	XGB E scp42	0.100000	4	0.081438	0.038341	4	0.095596	0.038341
			0.010000	274	0.000731	0.006368	361	0.009244	0.000035
			0.001000	274	0.000731	0.006368	—	—	—
			0.000100	13151	0.000011	0.000000	—	—	—
			0.000010	167458	0.000003	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	64414	DTR C scp42	0.100000	3	0.082691	0.062130	7	0.059712	0.001122
			0.010000	5	0.000722	0.034005	1093	0.008309	0.000000
			0.001000	5	0.000722	0.034005	—	—	—
			0.000100	21437	0.000035	0.000000	—	—	—
			0.000010	92779	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	64414	XGB E scp42	0.100000	7	0.070161	0.001122	7	0.059712	0.001122
			0.010000	1093	0.000080	0.000000	1093	0.008309	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	1093	0.000080	0.000000	—	—	—
			0.000100	1093	0.000080	0.000000	—	—	—
			0.000010	92779	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	70024	DTR C scp42	0.100000	3	0.076681	0.381252	23	0.050117	0.014617
			0.010000	78	0.006300	0.001207	598	0.009401	0.000000
			0.001000	1088	0.000682	0.000000	525441	0.000927	0.000000
			0.000100	24679	0.000028	0.000000	—	—	—
			0.000010	100887	0.000007	0.000000	—	—	—
			0.000001	525441	0.000001	0.000000	—	—	—
scp65	70024	XGB E scp42	0.100000	23	0.013640	0.014617	23	0.050117	0.014617
			0.010000	438	0.000657	0.000667	598	0.009401	0.000000
			0.001000	438	0.000657	0.000667	525441	0.000927	0.000000
			0.000100	5849	0.000055	0.000000	—	—	—
			0.000010	100887	0.000004	0.000000	—	—	—
			0.000001	525441	0.000001	0.000000	—	—	—
scp65	70336	DTR C scp42	0.100000	3	0.064610	0.590374	4	0.067780	0.003324
			0.010000	69	0.006300	0.001480	661	0.008724	0.000000
			0.001000	5459	0.000201	0.000000	—	—	—
			0.000100	50898	0.000021	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp65	70336	XGB E scp42	0.100000	69	0.021450	0.001480	4	0.067780	0.003324
			0.010000	542	0.000135	0.000922	661	0.008724	0.000000
			0.001000	542	0.000135	0.000922	—	—	—
			0.000100	5520	0.000098	0.000000	—	—	—
			0.000010	8718	0.000003	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	82153	DTR C scp42	0.100000	3	0.064610	0.354989	23	0.044373	0.054685
			0.010000	37	0.000136	0.008201	560	0.004102	0.000000
			0.001000	37	0.000136	0.008201	—	—	—
			0.000100	53	0.000041	0.001487	—	—	—
			0.000010	201111	0.000002	0.000000	—	—	—
			0.000001	513075	0.000001	0.000000	—	—	—
scp65	82153	XGB E scp42	0.100000	8	0.043266	0.347607	23	0.044373	0.054685
			0.010000	53	0.007867	0.001487	560	0.004102	0.000000
			0.001000	2996	0.000621	0.000000	—	—	—
			0.000100	16607	0.000075	0.000000	—	—	—
			0.000010	201111	0.000003	0.000000	—	—	—
			0.000001	513075	0.000001	0.000000	—	—	—
scp65	82443	DTR C scp42	0.100000	3	0.038658	0.051806	71	0.020557	0.011820
			0.010000	12	0.000722	0.042692	2570	0.006641	0.000000
			0.001000	12	0.000722	0.042692	436584	0.000943	0.000000
			0.000100	14424	0.000069	0.000000	—	—	—
			0.000010	145858	0.000005	0.000000	—	—	—
			0.000001	386342	0.000001	0.000000	—	—	—
scp65	82443	XGB E scp42	0.100000	12	0.075768	0.042692	71	0.020557	0.011820
			0.010000	116	0.008644	0.002383	2570	0.006641	0.000000
			0.001000	2570	0.000306	0.000000	436584	0.000943	0.000000
			0.000100	8115	0.000030	0.000000	—	—	—
			0.000010	145858	0.000005	0.000000	—	—	—
			0.000001	386342	0.000001	0.000000	—	—	—
scp65	88605	DTR C scp42	0.100000	3	0.038658	0.340888	8	0.033213	0.026436
			0.010000	8	0.000722	0.026436	608	0.008555	0.000366
			0.001000	8	0.000722	0.026436	—	—	—
			0.000100	18683	0.000060	0.000000	—	—	—
			0.000010	220666	0.000002	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
scp65	88605	XGB E scp42	0.100000	5	0.067689	0.258162	8	0.033213	0.026436
			0.010000	144	0.003877	0.024624	608	0.008555	0.000366
			0.001000	1715	0.000362	0.000000	—	—	—
			0.000100	29777	0.000031	0.000000	—	—	—
			0.000010	84888	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scp65	95465	DTR C scp42	0.100000	3	0.082691	0.652128	6	0.027055	0.229639
			0.010000	17	0.003334	0.170425	419	0.006041	0.000000
			0.001000	32	0.000136	0.007504	—	—	—
			0.000100	10671	0.000085	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scp65	95465	XGB E scp42	0.100000	17	0.020575	0.170425	6	0.027055	0.229639
			0.010000	22	0.003560	0.143729	419	0.006041	0.000000
			0.001000	10671	0.000043	0.000000	—	—	—
			0.000100	10671	0.000043	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpa4	20206	DTR C scp42	0.100000	3	0.093271	0.096107	37	0.049579	0.025270
			0.010000	5945	0.000180	0.000000	5945	0.002491	0.000000
			0.001000	5945	0.000180	0.000000	83608	0.000978	0.000000
			0.000100	13858	0.000069	0.000000	—	—	—
			0.000010	232382	0.000002	0.000000	—	—	—
			0.000001	359300	0.000001	0.000000	—	—	—
scpa4	20206	XGB E scp42	0.100000	37	0.024186	0.025270	37	0.049579	0.025270
			0.010000	5945	0.000142	0.000000	5945	0.002491	0.000000
			0.001000	5945	0.000142	0.000000	83608	0.000978	0.000000
			0.000100	13858	0.000041	0.000000	—	—	—
			0.000010	232382	0.000002	0.000000	—	—	—
			0.000001	359300	0.000001	0.000000	—	—	—
scpa4	31872	DTR C scp42	0.100000	3	0.082691	0.046685	21	0.066924	0.034057
			0.010000	78	0.006300	0.000621	78	0.006439	0.000621
			0.001000	952	0.000682	0.000000	19958	0.000769	0.000000
			0.000100	9803	0.000078	0.000000	—	—	—
			0.000010	255706	0.000002	0.000000	—	—	—
			0.000001	436872	0.000001	0.000000	—	—	—
scpa4	31872	XGB E scp42	0.100000	21	0.023196	0.034057	21	0.066924	0.034057
			0.010000	574	0.000032	0.000000	78	0.006439	0.000621
			0.001000	574	0.000032	0.000000	19958	0.000769	0.000000
			0.000100	574	0.000032	0.000000	—	—	—
			0.000010	255706	0.000002	0.000000	—	—	—
			0.000001	436872	0.000001	0.000000	—	—	—
scpa4	40563	DTR C scp42	0.100000	12	0.043126	0.033515	12	0.041526	0.033515
			0.010000	34	0.004795	0.002866	98	0.007641	0.000163
			0.001000	818	0.000682	0.000000	3921	0.000947	0.000000
			0.000100	100770	0.000007	0.000000	—	—	—
			0.000010	100770	0.000007	0.000000	—	—	—
			0.000001	832896	0.000000	0.000000	—	—	—
scpa4	40563	XGB E scp42	0.100000	12	0.075979	0.033515	12	0.041526	0.033515
			0.010000	98	0.007710	0.000163	98	0.007641	0.000163
			0.001000	818	0.000597	0.000000	3921	0.000947	0.000000
			0.000100	100770	0.000009	0.000000	—	—	—
			0.000010	100770	0.000009	0.000000	—	—	—
			0.000001	832896	0.000000	0.000000	—	—	—
scpa4	4516	DTR C scp42	0.100000	4	0.082691	0.072601	4	0.078863	0.072601
			0.010000	73	0.006300	0.000743	73	0.006894	0.000743

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	2202	0.000348	0.000000	93242	0.000452	0.000000
			0.000100	15464	0.000069	0.000000	—	—	—
			0.000010	93242	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpa4	4516	XGB E scp42	0.100000	4	0.092714	0.072601	4	0.078863	0.072601
			0.010000	26	0.007984	0.065036	73	0.006894	0.000743
			0.001000	2202	0.000360	0.000000	93242	0.000452	0.000000
			0.000100	15464	0.000041	0.000000	—	—	—
			0.000010	93242	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpa4	46197	DTR C scp42	0.100000	8	0.064610	0.090013	5	0.091107	0.143787
			0.010000	17	0.003334	0.001155	572	0.004202	0.000000
			0.001000	2440	0.000822	0.000000	164561	0.000617	0.000000
			0.000100	22569	0.000035	0.000000	—	—	—
			0.000010	132671	0.000005	0.000000	—	—	—
			0.000001	512103	0.000001	0.000000	—	—	—
scpa4	46197	XGB E scp42	0.100000	5	0.071295	0.143787	5	0.091107	0.143787
			0.010000	17	0.001086	0.001155	572	0.004202	0.000000
			0.001000	2440	0.000342	0.000000	164561	0.000617	0.000000
			0.000100	22569	0.000048	0.000000	—	—	—
			0.000010	132671	0.000003	0.000000	—	—	—
			0.000001	512103	0.000001	0.000000	—	—	—
scpa4	62924	DTR C scp42	0.100000	23	0.027368	0.063681	23	0.021731	0.063681
			0.010000	33	0.002215	0.000292	33	0.001489	0.000292
			0.001000	10644	0.000085	0.000000	10644	0.000560	0.000000
			0.000100	10644	0.000085	0.000000	—	—	—
			0.000010	610230	0.000001	0.000000	—	—	—
			0.000001	610230	0.000001	0.000000	—	—	—
scpa4	62924	XGB E scp42	0.100000	23	0.012083	0.063681	23	0.021731	0.063681
			0.010000	435	0.000635	0.000000	33	0.001489	0.000292
			0.001000	435	0.000635	0.000000	10644	0.000560	0.000000
			0.000100	10644	0.000069	0.000000	—	—	—
			0.000010	610230	0.000001	0.000000	—	—	—
			0.000001	610230	0.000001	0.000000	—	—	—
scpa4	72427	DTR C scp42	0.100000	3	0.064610	0.347092	26	0.018633	0.031332
			0.010000	559	0.006412	0.006223	889	0.007938	0.001665
			0.001000	889	0.000682	0.001665	17980	0.000870	0.000000
			0.000100	17980	0.000060	0.000000	—	—	—
			0.000010	200253	0.000002	0.000000	—	—	—
			0.000001	612099	0.000001	0.000000	—	—	—
scpa4	72427	XGB E scp42	0.100000	15	0.015256	0.218992	26	0.018633	0.031332
			0.010000	33	0.007128	0.022383	889	0.007938	0.001665
			0.001000	889	0.000490	0.001665	17980	0.000870	0.000000
			0.000100	8218	0.000030	0.000000	—	—	—
			0.000010	200253	0.000001	0.000000	—	—	—
			0.000001	200253	0.000001	0.000000	—	—	—
scpa4	79587	DTR C scp42	0.100000	14	0.054826	0.190415	33	0.097117	0.076963
			0.010000	109	0.007058	0.013011	315	0.008530	0.002141
			0.001000	67483	0.000019	0.000000	207401	0.000982	0.000000
			0.000100	67483	0.000019	0.000000	—	—	—
			0.000010	105944	0.000007	0.000000	—	—	—
			0.000001	890802	0.000000	0.000000	—	—	—
scpa4	79587	XGB E scp42	0.100000	14	0.016036	0.190415	33	0.097117	0.076963
			0.010000	22	0.000537	0.105076	315	0.008530	0.002141
			0.001000	22	0.000537	0.105076	207401	0.000982	0.000000
			0.000100	67483	0.000015	0.000000	—	—	—
			0.000010	105944	0.000006	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	890802	0.000000	0.000000	—	—	—
scpa4	82496	DTR C scp42	0.100000	4	0.038658	0.029849	4	0.098892	0.029849
			0.010000	311	0.001568	0.002788	311	0.009736	0.002788
			0.001000	3490	0.000727	0.000000	50560	0.000496	0.000000
			0.000100	30819	0.000028	0.000000	—	—	—
			0.000010	366694	0.000001	0.000000	—	—	—
			0.000001	366694	0.000001	0.000000	—	—	—
scpa4	82496	XGB E scp42	0.100000	4	0.093703	0.029849	4	0.098892	0.029849
			0.010000	311	0.001509	0.002788	311	0.009736	0.002788
			0.001000	406	0.000748	0.001339	50560	0.000496	0.000000
			0.000100	30819	0.000042	0.000000	—	—	—
			0.000010	366694	0.000001	0.000000	—	—	—
			0.000001	366694	0.000001	0.000000	—	—	—
scpa4	84917	DTR C scp42	0.100000	8	0.013186	0.008544	8	0.009093	0.008544
			0.010000	495	0.001623	0.000074	8	0.009093	0.008544
			0.001000	802	0.000682	0.000000	9374	0.000750	0.000000
			0.000100	384880	0.000001	0.000000	—	—	—
			0.000010	384880	0.000001	0.000000	—	—	—
			0.000001	384880	0.000001	0.000000	—	—	—
scpa4	84917	XGB E scp42	0.100000	4	0.083425	0.643664	8	0.009093	0.008544
			0.010000	495	0.000541	0.000074	8	0.009093	0.008544
			0.001000	495	0.000541	0.000074	9374	0.000750	0.000000
			0.000100	9374	0.000000	0.000000	—	—	—
			0.000010	9374	0.000000	0.000000	—	—	—
			0.000001	9374	0.000000	0.000000	—	—	—
scpb3	13133	DTR C scp42	0.100000	3	0.038658	0.588154	5	0.058029	0.038892
			0.010000	5	0.000722	0.038892	9662	0.009676	0.000000
			0.001000	5	0.000722	0.038892	—	—	—
			0.000100	10622	0.000085	0.000000	—	—	—
			0.000010	704667	0.000000	0.000000	—	—	—
			0.000001	704667	0.000000	0.000000	—	—	—
scpb3	13133	XGB E scp42	0.100000	10	0.071729	0.006609	5	0.058029	0.038892
			0.010000	314	0.002937	0.005896	9662	0.009676	0.000000
			0.001000	527	0.000496	0.004161	—	—	—
			0.000100	7182	0.000092	0.000000	—	—	—
			0.000010	704667	0.000000	0.000000	—	—	—
			0.000001	704667	0.000000	0.000000	—	—	—
scpb3	34257	DTR C scp42	0.100000	3	0.038658	0.400431	5	0.084194	0.195610
			0.010000	5	0.000722	0.195610	8013	0.009323	0.000000
			0.001000	5	0.000722	0.195610	—	—	—
			0.000100	20118	0.000045	0.000000	—	—	—
			0.000010	95214	0.000007	0.000000	—	—	—
			0.000001	806015	0.000000	0.000000	—	—	—
scpb3	34257	XGB E scp42	0.100000	12	0.077073	0.073876	5	0.084194	0.195610
			0.010000	457	0.000517	0.000000	8013	0.009323	0.000000
			0.001000	457	0.000517	0.000000	—	—	—
			0.000100	8013	0.000025	0.000000	—	—	—
			0.000010	95214	0.000010	0.000000	—	—	—
			0.000001	806015	0.000000	0.000000	—	—	—
scpb3	4964	DTR C scp42	0.100000	3	0.038658	0.387150	6	0.032844	0.019317
			0.010000	6	0.000722	0.019317	7318	0.005992	0.000000
			0.001000	6	0.000722	0.019317	—	—	—
			0.000100	57996	0.000021	0.000000	—	—	—
			0.000010	98429	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpb3	4964	XGB E scp42	0.100000	6	0.098222	0.019317	6	0.032844	0.019317
			0.010000	1173	0.000059	0.000000	7318	0.005992	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	1173	0.000059	0.000000	—	—	—
			0.000100	1173	0.000059	0.000000	—	—	—
			0.000010	70917	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpb3	66361	DTR C scp42	0.100000	3	0.038658	0.124344	57	0.092362	0.061239
			0.010000	6	0.000722	0.093677	2744	0.007861	0.000000
			0.001000	6	0.000722	0.093677	—	—	—
			0.000100	54847	0.000021	0.000000	—	—	—
			0.000010	206217	0.000002	0.000000	—	—	—
			0.000001	342279	0.000001	0.000000	—	—	—
scpb3	66361	XGB E scp42	0.100000	6	0.079251	0.093677	57	0.092362	0.061239
			0.010000	75	0.006391	0.003696	2744	0.007861	0.000000
			0.001000	1123	0.000459	0.000000	—	—	—
			0.000100	54847	0.000015	0.000000	—	—	—
			0.000010	206217	0.000003	0.000000	—	—	—
			0.000001	342279	0.000001	0.000000	—	—	—
scpb3	71918	DTR C scp42	0.100000	3	0.038658	0.303578	9	0.053349	0.075953
			0.010000	5	0.000722	0.209618	739	0.007752	0.000000
			0.001000	5	0.000722	0.209618	—	—	—
			0.000100	23759	0.000035	0.000000	—	—	—
			0.000010	86646	0.000007	0.000000	—	—	—
			0.000001	493464	0.000001	0.000000	—	—	—
scpb3	71918	XGB E scp42	0.100000	5	0.071295	0.209618	9	0.053349	0.075953
			0.010000	185	0.002034	0.001615	739	0.007752	0.000000
			0.001000	739	0.000543	0.000000	—	—	—
			0.000100	23759	0.000044	0.000000	—	—	—
			0.000010	125643	0.000004	0.000000	—	—	—
			0.000001	493464	0.000001	0.000000	—	—	—
scpb3	8320	DTR C scp42	0.100000	3	0.038658	0.417638	8	0.057808	0.184216
			0.010000	8	0.000722	0.184216	3866	0.008025	0.000000
			0.001000	8	0.000722	0.184216	—	—	—
			0.000100	9993	0.000078	0.000000	—	—	—
			0.000010	510116	0.000001	0.000000	—	—	—
			0.000001	510116	0.000001	0.000000	—	—	—
scpb3	8320	XGB E scp42	0.100000	8	0.082684	0.184216	8	0.057808	0.184216
			0.010000	3866	0.000480	0.000000	3866	0.008025	0.000000
			0.001000	3866	0.000480	0.000000	—	—	—
			0.000100	9993	0.000033	0.000000	—	—	—
			0.000010	510116	0.000001	0.000000	—	—	—
			0.000001	510116	0.000001	0.000000	—	—	—
scpb3	8536	DTR C scp42	0.100000	3	0.038658	0.471312	4	0.082857	0.335098
			0.010000	5	0.000722	0.230255	136	0.006803	0.000000
			0.001000	5	0.000722	0.230255	—	—	—
			0.000100	19956	0.000045	0.000000	—	—	—
			0.000010	388100	0.000001	0.000000	—	—	—
			0.000001	388100	0.000001	0.000000	—	—	—
scpb3	8536	XGB E scp42	0.100000	4	0.092714	0.335098	4	0.082857	0.335098
			0.010000	17	0.001086	0.010739	136	0.006803	0.000000
			0.001000	8007	0.000028	0.000000	—	—	—
			0.000100	8007	0.000028	0.000000	—	—	—
			0.000010	388100	0.000001	0.000000	—	—	—
			0.000001	388100	0.000001	0.000000	—	—	—
scpb3	94506	DTR C scp42	0.100000	3	0.038658	0.124261	42	0.085618	0.081389
			0.010000	42	0.000041	0.081389	1956	0.006703	0.000000
			0.001000	42	0.000041	0.081389	—	—	—
			0.000100	42	0.000041	0.081389	—	—	—
			0.000010	252739	0.000002	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	—	—	—	—	—	—
scpb3	94506	XGB E scp42	0.100000	42	0.023654	0.081389	42	0.085618	0.081389
			0.010000	342	0.001576	0.001703	1956	0.006703	0.000000
			0.001000	627	0.000522	0.000430	—	—	—
			0.000100	252739	0.000002	0.000000	—	—	—
			0.000010	252739	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpb3	97529	DTR C scp42	0.100000	3	0.038658	0.241430	18	0.096002	0.087604
			0.010000	5	0.000722	0.202311	1708	0.006748	0.000000
			0.001000	5	0.000722	0.202311	—	—	—
			0.000100	45	0.000041	0.014720	—	—	—
			0.000010	133704	0.000005	0.000000	—	—	—
			0.000001	955240	0.000000	0.000000	—	—	—
scpb3	97529	XGB E scp42	0.100000	5	0.071295	0.202311	18	0.096002	0.087604
			0.010000	18	0.002435	0.087604	1708	0.006748	0.000000
			0.001000	1050	0.000881	0.000000	—	—	—
			0.000100	67983	0.000014	0.000000	—	—	—
			0.000010	133704	0.000005	0.000000	—	—	—
			0.000001	955240	0.000000	0.000000	—	—	—
scpb3	9925	DTR C scp42	0.100000	3	0.038658	0.674091	5	0.074105	0.229659
			0.010000	5	0.000722	0.229659	870	0.008640	0.000000
			0.001000	5	0.000722	0.229659	—	—	—
			0.000100	56	0.000041	0.002009	—	—	—
			0.000010	107579	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpb3	9925	XGB E scp42	0.100000	4	0.093703	0.580180	5	0.074105	0.229659
			0.010000	13	0.000437	0.117951	870	0.008640	0.000000
			0.001000	13	0.000437	0.117951	—	—	—
			0.000100	47961	0.000022	0.000000	—	—	—
			0.000010	107579	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	1049	DTR C scp42	0.100000	12	0.013186	0.218074	4	0.092296	0.291538
			0.010000	306	0.001568	0.004460	592	0.005362	0.001007
			0.001000	1278	0.000636	0.000000	26133	0.000856	0.000000
			0.000100	11247	0.000085	0.000000	—	—	—
			0.000010	132059	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	1049	XGB E scp42	0.100000	4	0.092657	0.291538	4	0.092296	0.291538
			0.010000	16	0.001099	0.046587	592	0.005362	0.001007
			0.001000	2017	0.000636	0.000000	26133	0.000856	0.000000
			0.000100	9710	0.000039	0.000000	—	—	—
			0.000010	132059	0.000001	0.000000	—	—	—
			0.000001	132059	0.000001	0.000000	—	—	—
scpc1	12401	DTR C scp42	0.100000	11	0.013186	0.020792	11	0.040829	0.020792
			0.010000	17	0.003334	0.018825	309	0.009211	0.003284
			0.001000	4108	0.000283	0.000000	8552	0.000839	0.000000
			0.000100	23471	0.000035	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	12401	XGB E scp42	0.100000	4	0.092657	0.208861	11	0.040829	0.020792
			0.010000	17	0.001101	0.018825	309	0.009211	0.003284
			0.001000	4108	0.000410	0.000000	8552	0.000839	0.000000
			0.000100	7424	0.000079	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	29296	DTR C scp42	0.100000	5	0.025506	0.028339	5	0.067407	0.028339
			0.010000	459	0.002238	0.002471	459	0.006107	0.002471

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	1463	0.000636	0.000000	1463	0.000874	0.000000
			0.000100	116453	0.000006	0.000000	—	—	—
			0.000010	116453	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	29296	XGB E scp42	0.100000	14	0.016695	0.020499	5	0.067407	0.028339
			0.010000	459	0.000517	0.002471	459	0.006107	0.002471
			0.001000	459	0.000517	0.002471	1463	0.000874	0.000000
			0.000100	116453	0.000006	0.000000	—	—	—
			0.000010	116453	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	3065	DTR C scp42	0.100000	4	0.038658	0.017972	38	0.025318	0.011599
			0.010000	99	0.007058	0.006657	99	0.009924	0.006657
			0.001000	228	0.000398	0.004878	10287	0.000752	0.000000
			0.000100	10287	0.000078	0.000000	—	—	—
			0.000010	205869	0.000002	0.000000	—	—	—
			0.000001	396526	0.000001	0.000000	—	—	—
scpc1	3065	XGB E scp42	0.100000	38	0.024644	0.011599	38	0.025318	0.011599
			0.010000	99	0.008240	0.006657	99	0.009924	0.006657
			0.001000	302	0.000912	0.004267	10287	0.000752	0.000000
			0.000100	10287	0.000051	0.000000	—	—	—
			0.000010	205869	0.000002	0.000000	—	—	—
			0.000001	396526	0.000001	0.000000	—	—	—
scpc1	35343	DTR C scp42	0.100000	15	0.043227	0.081675	15	0.052878	0.081675
			0.010000	406	0.002333	0.005498	21	0.009787	0.006272
			0.001000	778	0.000682	0.000000	6065	0.000501	0.000000
			0.000100	405613	0.000001	0.000000	—	—	—
			0.000010	405613	0.000001	0.000000	—	—	—
			0.000001	405613	0.000001	0.000000	—	—	—
scpc1	35343	XGB E scp42	0.100000	15	0.009710	0.081675	15	0.052878	0.081675
			0.010000	15	0.009710	0.081675	21	0.009787	0.006272
			0.001000	778	0.000604	0.000000	6065	0.000501	0.000000
			0.000100	6065	0.000024	0.000000	—	—	—
			0.000010	405613	0.000001	0.000000	—	—	—
			0.000001	405613	0.000001	0.000000	—	—	—
scpc1	40226	DTR C scp42	0.100000	14	0.043227	0.062633	14	0.013823	0.062633
			0.010000	17	0.003334	0.014871	17	0.009979	0.014871
			0.001000	3087	0.000385	0.000000	67668	0.000662	0.000000
			0.000100	22002	0.000035	0.000000	—	—	—
			0.000010	86545	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	40226	XGB E scp42	0.100000	14	0.017350	0.062633	14	0.013823	0.062633
			0.010000	3087	0.000569	0.000000	17	0.009979	0.014871
			0.001000	3087	0.000569	0.000000	67668	0.000662	0.000000
			0.000100	5605	0.000078	0.000000	—	—	—
			0.000010	86545	0.000004	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	54123	DTR C scp42	0.100000	3	0.064610	0.102706	44	0.001232	0.000146
			0.010000	44	0.002215	0.000146	44	0.001232	0.000146
			0.001000	4626	0.000266	0.000000	59261	0.000300	0.000000
			0.000100	21389	0.000035	0.000000	—	—	—
			0.000010	776521	0.000000	0.000000	—	—	—
			0.000001	776521	0.000000	0.000000	—	—	—
scpc1	54123	XGB E scp42	0.100000	44	0.026683	0.000146	44	0.001232	0.000146
			0.010000	4626	0.000328	0.000000	44	0.001232	0.000146
			0.001000	4626	0.000328	0.000000	59261	0.000300	0.000000
			0.000100	21389	0.000046	0.000000	—	—	—
			0.000010	776521	0.000000	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	776521	0.000000	0.000000	—	—	—
scpc1	64402	DTR C scp42	0.100000	3	0.082691	0.025613	87	0.037151	0.015709
			0.010000	99	0.007058	0.000879	1421	0.001172	0.000000
			0.001000	1421	0.000636	0.000000	48892	0.000727	0.000000
			0.000100	25878	0.000028	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	64402	XGB E scp42	0.100000	87	0.020647	0.015709	87	0.037151	0.015709
			0.010000	1421	0.000120	0.000000	1421	0.001172	0.000000
			0.001000	1421	0.000120	0.000000	48892	0.000727	0.000000
			0.000100	25878	0.000040	0.000000	—	—	—
			0.000010	81535	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpc1	75033	DTR C scp42	0.100000	3	0.054172	0.012717	77	0.033678	0.011976
			0.010000	102	0.007058	0.006179	454	0.008675	0.003176
			0.001000	364	0.000606	0.005519	18064	0.000828	0.000000
			0.000100	15288	0.000069	0.000000	—	—	—
			0.000010	320173	0.000002	0.000000	—	—	—
			0.000001	600280	0.000001	0.000000	—	—	—
scpc1	75033	XGB E scp42	0.100000	77	0.019762	0.011976	77	0.033678	0.011976
			0.010000	364	0.002731	0.005519	454	0.008675	0.003176
			0.001000	454	0.000517	0.003176	18064	0.000828	0.000000
			0.000100	6946	0.000050	0.000000	—	—	—
			0.000010	74357	0.000010	0.000000	—	—	—
			0.000001	600280	0.000001	0.000000	—	—	—
scpc1	97250	DTR C scp42	0.100000	10	0.056393	0.141088	10	0.035548	0.141088
			0.010000	84	0.006300	0.005621	768	0.003874	0.000000
			0.001000	768	0.000811	0.000000	6870	0.000778	0.000000
			0.000100	47354	0.000025	0.000000	—	—	—
			0.000010	86546	0.000007	0.000000	—	—	—
			0.000001	573208	0.000001	0.000000	—	—	—
scpc1	97250	XGB E scp42	0.100000	10	0.070793	0.141088	10	0.035548	0.141088
			0.010000	97	0.008234	0.005493	768	0.003874	0.000000
			0.001000	768	0.000443	0.000000	6870	0.000778	0.000000
			0.000100	47354	0.000020	0.000000	—	—	—
			0.000010	86546	0.000005	0.000000	—	—	—
			0.000001	573208	0.000001	0.000000	—	—	—
scpd1	12316	DTR C scp42	0.100000	3	0.038658	0.059258	12	0.051945	0.016503
			0.010000	12	0.000722	0.016503	4071	0.008755	0.000000
			0.001000	12	0.000722	0.016503	—	—	—
			0.000100	25163	0.000028	0.000000	—	—	—
			0.000010	93186	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	12316	XGB E scp42	0.100000	12	0.032007	0.016503	12	0.051945	0.016503
			0.010000	153	0.003473	0.012179	4071	0.008755	0.000000
			0.001000	406	0.000670	0.004247	—	—	—
			0.000100	9779	0.000054	0.000000	—	—	—
			0.000010	93186	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	13826	DTR C scp42	0.100000	3	0.038658	0.260261	12	0.082157	0.102477
			0.010000	12	0.000722	0.102477	3580	0.005288	0.000000
			0.001000	12	0.000722	0.102477	—	—	—
			0.000100	18675	0.000060	0.000000	—	—	—
			0.000010	149685	0.000005	0.000000	—	—	—
			0.000001	533386	0.000001	0.000000	—	—	—
scpd1	13826	XGB E scp42	0.100000	12	0.082026	0.102477	12	0.082157	0.102477
			0.010000	130	0.005303	0.001321	3580	0.005288	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	561	0.000572	0.000272	—	—	—
			0.000100	149685	0.000003	0.000000	—	—	—
			0.000010	149685	0.000003	0.000000	—	—	—
			0.000001	533386	0.000001	0.000000	—	—	—
scpd1	23931	DTR C scp42	0.100000	3	0.038658	0.065585	27	0.092350	0.021526
			0.010000	54	0.000041	0.008832	2207	0.006289	0.000000
			0.001000	54	0.000041	0.008832	—	—	—
			0.000100	54	0.000041	0.008832	—	—	—
			0.000010	97034	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	23931	XGB E scp42	0.100000	25	0.023196	0.048665	27	0.092350	0.021526
			0.010000	213	0.001067	0.006583	2207	0.006289	0.000000
			0.001000	253	0.000623	0.002380	—	—	—
			0.000100	26199	0.000042	0.000000	—	—	—
			0.000010	97034	0.000004	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	26284	DTR C scp42	0.100000	3	0.038658	0.369192	8	0.055505	0.016729
			0.010000	8	0.000722	0.016729	1768	0.007893	0.000000
			0.001000	8	0.000722	0.016729	—	—	—
			0.000100	72113	0.000013	0.000000	—	—	—
			0.000010	153614	0.000005	0.000000	—	—	—
			0.000001	524113	0.000001	0.000000	—	—	—
scpd1	26284	XGB E scp42	0.100000	8	0.086416	0.016729	8	0.055505	0.016729
			0.010000	138	0.005441	0.003015	1768	0.007893	0.000000
			0.001000	402	0.000670	0.000000	—	—	—
			0.000100	72113	0.000007	0.000000	—	—	—
			0.000010	72113	0.000007	0.000000	—	—	—
			0.000001	524113	0.000001	0.000000	—	—	—
scpd1	44691	DTR C scp42	0.100000	3	0.038658	0.569987	7	0.090705	0.526313
			0.010000	7	0.000722	0.526313	9796	0.007974	0.000000
			0.001000	7	0.000722	0.526313	—	—	—
			0.000100	54	0.000041	0.035017	—	—	—
			0.000010	167535	0.000005	0.000000	—	—	—
			0.000001	877177	0.000000	0.000000	—	—	—
scpd1	44691	XGB E scp42	0.100000	7	0.076837	0.526313	7	0.090705	0.526313
			0.010000	20	0.002018	0.165522	9796	0.007974	0.000000
			0.001000	1480	0.000383	0.000000	—	—	—
			0.000100	9228	0.000036	0.000000	—	—	—
			0.000010	78720	0.000005	0.000000	—	—	—
			0.000001	167535	0.000001	0.000000	—	—	—
scpd1	45107	DTR C scp42	0.100000	3	0.038658	0.687723	4	0.082317	0.102146
			0.010000	7	0.000722	0.090679	10462	0.005442	0.000000
			0.001000	7	0.000722	0.090679	—	—	—
			0.000100	55	0.000041	0.032128	—	—	—
			0.000010	122881	0.000006	0.000000	—	—	—
			0.000001	714485	0.000000	0.000000	—	—	—
scpd1	45107	XGB E scp42	0.100000	7	0.076837	0.090679	4	0.082317	0.102146
			0.010000	37	0.008146	0.035119	10462	0.005442	0.000000
			0.001000	4738	0.000642	0.000000	—	—	—
			0.000100	10462	0.000086	0.000000	—	—	—
			0.000010	122881	0.000005	0.000000	—	—	—
			0.000001	714485	0.000000	0.000000	—	—	—
scpd1	45796	DTR C scp42	0.100000	3	0.038658	0.143832	22	0.098519	0.123751
			0.010000	32	0.000136	0.072935	1258	0.006181	0.000000
			0.001000	32	0.000136	0.072935	—	—	—
			0.000100	41	0.000041	0.070585	—	—	—
			0.000010	132801	0.000005	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	779093	0.000000	0.000000	—	—	—
scpd1	45796	XGB E scp42	0.100000	22	0.024395	0.123751	22	0.098519	0.123751
			0.010000	51	0.003920	0.005479	1258	0.006181	0.000000
			0.001000	1258	0.000559	0.000000	—	—	—
			0.000100	15724	0.000045	0.000000	—	—	—
			0.000010	132801	0.000003	0.000000	—	—	—
			0.000001	779093	0.000000	0.000000	—	—	—
scpd1	70795	DTR C scp42	0.100000	3	0.038658	0.242844	7	0.057856	0.088443
			0.010000	7	0.000722	0.088443	6363	0.009042	0.000000
			0.001000	7	0.000722	0.088443	—	—	—
			0.000100	46	0.000041	0.008465	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	70795	XGB E scp42	0.100000	7	0.088498	0.088443	7	0.057856	0.088443
			0.010000	123	0.007457	0.004657	6363	0.009042	0.000000
			0.001000	681	0.000513	0.003102	—	—	—
			0.000100	47371	0.000018	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
scpd1	73667	DTR C scp42	0.100000	3	0.038658	0.011801	42	0.036840	0.003338
			0.010000	42	0.000041	0.003338	2566	0.006134	0.000000
			0.001000	42	0.000041	0.003338	—	—	—
			0.000100	42	0.000041	0.003338	—	—	—
			0.000010	101661	0.000007	0.000000	—	—	—
			0.000001	360467	0.000001	0.000000	—	—	—
scpd1	73667	XGB E scp42	0.100000	42	0.022094	0.003338	42	0.036840	0.003338
			0.010000	1085	0.000087	0.000000	2566	0.006134	0.000000
			0.001000	1085	0.000087	0.000000	—	—	—
			0.000100	1085	0.000087	0.000000	—	—	—
			0.000010	149893	0.000003	0.000000	—	—	—
			0.000001	360467	0.000001	0.000000	—	—	—
scpd1	84688	DTR C scp42	0.100000	3	0.038658	0.043663	90	0.048624	0.018613
			0.010000	90	0.006300	0.018613	9702	0.003418	0.000000
			0.001000	1906	0.000476	0.000000	—	—	—
			0.000100	242759	0.000002	0.000000	—	—	—
			0.000010	242759	0.000002	0.000000	—	—	—
			0.000001	486119	0.000001	0.000000	—	—	—
scpd1	84688	XGB E scp42	0.100000	90	0.018810	0.018613	90	0.048624	0.018613
			0.010000	160	0.003430	0.007808	9702	0.003418	0.000000
			0.001000	424	0.000670	0.000169	—	—	—
			0.000100	9702	0.000057	0.000000	—	—	—
			0.000010	242759	0.000002	0.000000	—	—	—
			0.000001	486119	0.000001	0.000000	—	—	—
scpd5	11156	DTR C scp42	0.100000	3	0.038658	0.513077	19	0.079667	0.084244
			0.010000	9	0.000722	0.096530	681	0.007568	0.000000
			0.001000	9	0.000722	0.096530	—	—	—
			0.000100	10759	0.000085	0.000000	—	—	—
			0.000010	121323	0.000006	0.000000	—	—	—
			0.000001	414577	0.000001	0.000000	—	—	—
scpd5	11156	XGB E scp42	0.100000	9	0.053672	0.096530	19	0.079667	0.084244
			0.010000	297	0.003492	0.005137	681	0.007568	0.000000
			0.001000	681	0.000661	0.000000	—	—	—
			0.000100	10759	0.000047	0.000000	—	—	—
			0.000010	121323	0.000004	0.000000	—	—	—
			0.000001	414577	0.000001	0.000000	—	—	—
scpd5	17148	DTR C scp42	0.100000	3	0.038658	0.017675	52	0.056630	0.014560
			0.010000	52	0.000041	0.014560	7109	0.009297	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	52	0.000041	0.014560	—	—	—
			0.000100	52	0.000041	0.014560	—	—	—
			0.000010	554500	0.000001	0.000000	—	—	—
			0.000001	554500	0.000001	0.000000	—	—	—
scpd5	17148	XGB E scp42	0.100000	52	0.013244	0.014560	52	0.056630	0.014560
			0.010000	2245	0.000272	0.000000	7109	0.009297	0.000000
			0.001000	2245	0.000272	0.000000	—	—	—
			0.000100	7567	0.000020	0.000000	—	—	—
			0.000010	8236	0.000009	0.000000	—	—	—
			0.000001	554500	0.000001	0.000000	—	—	—
scpd5	47174	DTR C scp42	0.100000	3	0.038658	0.117445	32	0.050378	0.007340
			0.010000	9	0.000722	0.062899	984	0.005703	0.000000
			0.001000	9	0.000722	0.062899	—	—	—
			0.000100	24806	0.000028	0.000000	—	—	—
			0.000010	167789	0.000005	0.000000	—	—	—
			0.000001	412629	0.000001	0.000000	—	—	—
scpd5	47174	XGB E scp42	0.100000	9	0.051501	0.062899	32	0.050378	0.007340
			0.010000	16	0.000131	0.037715	984	0.005703	0.000000
			0.001000	16	0.000131	0.037715	—	—	—
			0.000100	24806	0.000029	0.000000	—	—	—
			0.000010	167789	0.000004	0.000000	—	—	—
			0.000001	412629	0.000001	0.000000	—	—	—
scpd5	52090	DTR C scp42	0.100000	3	0.038658	0.206467	9	0.078602	0.109120
			0.010000	9	0.000722	0.109120	2050	0.009947	0.000000
			0.001000	9	0.000722	0.109120	—	—	—
			0.000100	16267	0.000069	0.000000	—	—	—
			0.000010	110423	0.000006	0.000000	—	—	—
			0.000001	422463	0.000001	0.000000	—	—	—
scpd5	52090	XGB E scp42	0.100000	9	0.055233	0.109120	9	0.078602	0.109120
			0.010000	173	0.003432	0.002174	2050	0.009947	0.000000
			0.001000	1343	0.000464	0.000000	—	—	—
			0.000100	16267	0.000075	0.000000	—	—	—
			0.000010	110423	0.000006	0.000000	—	—	—
			0.000001	422463	0.000001	0.000000	—	—	—
scpd5	54807	DTR C scp42	0.100000	3	0.038658	0.144776	34	0.052549	0.012587
			0.010000	11	0.000722	0.096262	3303	0.004577	0.000000
			0.001000	11	0.000722	0.096262	—	—	—
			0.000100	82584	0.000011	0.000000	—	—	—
			0.000010	318445	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd5	54807	XGB E scp42	0.100000	11	0.041059	0.096262	34	0.052549	0.012587
			0.010000	292	0.001858	0.005137	3303	0.004577	0.000000
			0.001000	415	0.000754	0.002822	—	—	—
			0.000100	82584	0.000012	0.000000	—	—	—
			0.000010	318445	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd5	59075	DTR C scp42	0.100000	3	0.038658	0.515834	7	0.060496	0.221904
			0.010000	7	0.000722	0.221904	2179	0.009486	0.000000
			0.001000	7	0.000722	0.221904	—	—	—
			0.000100	45	0.000041	0.038982	—	—	—
			0.000010	96521	0.000007	0.000000	—	—	—
			0.000001	677673	0.000000	0.000000	—	—	—
scpd5	59075	XGB E scp42	0.100000	7	0.094340	0.221904	7	0.060496	0.221904
			0.010000	25	0.007954	0.053436	2179	0.009486	0.000000
			0.001000	1280	0.000470	0.000000	—	—	—
			0.000100	17029	0.000096	0.000000	—	—	—
			0.000010	73259	0.000007	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	677673	0.000000	0.000000	—	—	—
scpd5	76943	DTR C scp42	0.100000	3	0.038658	0.957897	4	0.080715	0.269357
			0.010000	5	0.000722	0.151309	3758	0.008965	0.000000
			0.001000	5	0.000722	0.151309	—	—	—
			0.000100	54	0.000041	0.001702	—	—	—
			0.000010	95339	0.000007	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd5	76943	XGB E scp42	0.100000	5	0.068878	0.151309	4	0.080715	0.269357
			0.010000	9	0.007320	0.029845	3758	0.008965	0.000000
			0.001000	2109	0.000480	0.000000	—	—	—
			0.000100	95339	0.000005	0.000000	—	—	—
			0.000010	95339	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd5	77970	DTR C scp42	0.100000	3	0.038658	0.006118	48	0.039468	0.004996
			0.010000	48	0.000041	0.004996	6957	0.009878	0.000000
			0.001000	48	0.000041	0.004996	—	—	—
			0.000100	48	0.000041	0.004996	—	—	—
			0.000010	177471	0.000005	0.000000	—	—	—
			0.000001	388764	0.000001	0.000000	—	—	—
scpd5	77970	XGB E scp42	0.100000	48	0.009390	0.004996	48	0.039468	0.004996
			0.010000	48	0.009390	0.004996	6957	0.009878	0.000000
			0.001000	598	0.000052	0.002670	—	—	—
			0.000100	598	0.000052	0.002670	—	—	—
			0.000010	78798	0.000006	0.000000	—	—	—
			0.000001	388764	0.000001	0.000000	—	—	—
scpd5	9743	DTR C scp42	0.100000	3	0.038658	0.541312	4	0.088545	0.335135
			0.010000	7	0.000722	0.040412	4183	0.007007	0.000000
			0.001000	7	0.000722	0.040412	—	—	—
			0.000100	53	0.000041	0.029549	—	—	—
			0.000010	132662	0.000005	0.000000	—	—	—
			0.000001	836628	0.000000	0.000000	—	—	—
scpd5	9743	XGB E scp42	0.100000	4	0.092657	0.335135	4	0.088545	0.335135
			0.010000	53	0.008812	0.029549	4183	0.007007	0.000000
			0.001000	4183	0.000619	0.000000	—	—	—
			0.000100	50749	0.000016	0.000000	—	—	—
			0.000010	132662	0.000005	0.000000	—	—	—
			0.000001	836628	0.000000	0.000000	—	—	—
scpd5	98757	DTR C scp42	0.100000	3	0.038658	0.452571	28	0.064322	0.012467
			0.010000	5	0.000722	0.413809	3116	0.007267	0.000000
			0.001000	5	0.000722	0.413809	—	—	—
			0.000100	34615	0.000028	0.000000	—	—	—
			0.000010	125370	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
scpd5	98757	XGB E scp42	0.100000	6	0.074827	0.238271	28	0.064322	0.012467
			0.010000	10	0.007446	0.133399	3116	0.007267	0.000000
			0.001000	994	0.000145	0.000000	—	—	—
			0.000100	6810	0.000063	0.000000	—	—	—
			0.000010	125370	0.000002	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
sko56	11084	DTR C scp42	0.100000	2	0.082691	0.429007	3	0.081701	0.052466
			0.010000	133	0.004777	0.003940	595	0.007707	0.002088
			0.001000	837	0.000682	0.000804	7515	0.000849	0.000000
			0.000100	20649	0.000035	0.000000	—	—	—
			0.000010	181197	0.000005	0.000000	—	—	—
			0.000001	500100	0.000001	0.000000	—	—	—
sko56	11084	XGB E scp42	0.100000	6	0.058484	0.025089	3	0.081701	0.052466
			0.010000	17	0.000647	0.022927	595	0.007707	0.002088

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	17	0.000647	0.022927	7515	0.000849	0.000000
			0.000100	7515	0.000044	0.000000	—	—	—
			0.000010	181197	0.000001	0.000000	—	—	—
			0.000001	181197	0.000001	0.000000	—	—	—
sko56	22727	DTR C scp42	0.100000	2	0.082691	0.777605	4	0.080734	0.332709
			0.010000	394	0.002333	0.000669	35	0.006340	0.006646
			0.001000	1357	0.000636	0.000000	2482	0.000576	0.000000
			0.000100	68554	0.000016	0.000000	—	—	—
			0.000010	—	—	—	—	—	—
			0.000001	—	—	—	—	—	—
sko56	22727	XGB E scp42	0.100000	4	0.092657	0.332709	4	0.080734	0.332709
			0.010000	14	-0.003185	0.117303	35	0.006340	0.006646
			0.001000	14	-0.003185	0.117303	2482	0.000576	0.000000
			0.000100	14	-0.003185	0.117303	—	—	—
			0.000010	14	-0.003185	0.117303	—	—	—
			0.000001	14	-0.003185	0.117303	—	—	—
sko56	23382	DTR C scp42	0.100000	2	0.082691	0.064542	67	0.024863	0.008037
			0.010000	479	0.001623	0.001531	479	0.007412	0.001531
			0.001000	1324	0.000636	0.000000	52660	0.000731	0.000000
			0.000100	12747	0.000085	0.000000	—	—	—
			0.000010	88031	0.000007	0.000000	—	—	—
			0.000001	960122	0.000000	0.000000	—	—	—
sko56	23382	XGB E scp42	0.100000	67	0.021596	0.008037	67	0.024863	0.008037
			0.010000	234	0.003154	0.005674	479	0.007412	0.001531
			0.001000	479	0.000579	0.001531	52660	0.000731	0.000000
			0.000100	12747	0.000028	0.000000	—	—	—
			0.000010	88031	0.000006	0.000000	—	—	—
			0.000001	960122	0.000000	0.000000	—	—	—
sko56	25873	DTR C scp42	0.100000	2	0.038658	0.073118	10	0.049377	0.046658
			0.010000	120	0.007058	0.014511	468	0.004803	0.001236
			0.001000	686	0.000811	0.000144	82261	0.000785	0.000000
			0.000100	82261	0.000011	0.000000	—	—	—
			0.000010	154368	0.000005	0.000000	—	—	—
			0.000001	431101	0.000001	0.000000	—	—	—
sko56	25873	XGB E scp42	0.100000	10	0.074524	0.046658	10	0.049377	0.046658
			0.010000	120	0.008316	0.014511	468	0.004803	0.001236
			0.001000	468	0.000586	0.001236	82261	0.000785	0.000000
			0.000100	6788	0.000067	0.000000	—	—	—
			0.000010	154368	0.000003	0.000000	—	—	—
			0.000001	431101	0.000001	0.000000	—	—	—
sko56	50686	DTR C scp42	0.100000	2	0.082691	0.297066	5	0.091925	0.145474
			0.010000	448	0.002333	0.000774	448	0.005213	0.000774
			0.001000	4397	0.000266	0.000000	37435	0.000805	0.000000
			0.000100	10320	0.000078	0.000000	—	—	—
			0.000010	146090	0.000005	0.000000	—	—	—
			0.000001	391558	0.000001	0.000000	—	—	—
sko56	50686	XGB E scp42	0.100000	15	0.015985	0.050978	5	0.091925	0.145474
			0.010000	448	0.000703	0.000774	448	0.005213	0.000774
			0.001000	448	0.000703	0.000774	37435	0.000805	0.000000
			0.000100	6598	0.000016	0.000000	—	—	—
			0.000010	146090	0.000004	0.000000	—	—	—
			0.000001	391558	0.000001	0.000000	—	—	—
sko56	55924	DTR C scp42	0.100000	2	0.064610	0.159902	7	0.080867	0.035372
			0.010000	108	0.007058	0.003195	408	0.008657	0.001976
			0.001000	790	0.000682	0.000000	4235	0.000927	0.000000
			0.000100	32319	0.000028	0.000000	—	—	—
			0.000010	698055	0.000000	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	698055	0.000000	0.000000	—	—	—
sko56	55924	XGB E scp42	0.100000	4	0.092657	0.117217	7	0.080867	0.035372
			0.010000	408	0.001570	0.001976	408	0.008657	0.001976
			0.001000	790	0.000477	0.000000	4235	0.000927	0.000000
			0.000100	32319	0.000036	0.000000	—	—	—
			0.000010	74018	0.000010	0.000000	—	—	—
			0.000001	698055	0.000000	0.000000	—	—	—
sko56	73203	DTR C scp42	0.100000	2	0.093271	0.330212	4	0.060325	0.034661
			0.010000	430	0.002333	0.005457	430	0.008877	0.005457
			0.001000	951	0.000682	0.000510	18598	0.000886	0.000000
			0.000100	11754	0.000085	0.000000	—	—	—
			0.000010	445945	0.000001	0.000000	—	—	—
			0.000001	445945	0.000001	0.000000	—	—	—
sko56	73203	XGB E scp42	0.100000	40	0.024862	0.009001	4	0.060325	0.034661
			0.010000	430	0.001361	0.005457	430	0.008877	0.005457
			0.001000	584	0.000509	0.001036	18598	0.000886	0.000000
			0.000100	6986	0.000095	0.000000	—	—	—
			0.000010	445945	0.000001	0.000000	—	—	—
			0.000001	445945	0.000001	0.000000	—	—	—
sko56	77695	DTR C scp42	0.100000	2	0.082691	0.389232	3	0.097353	0.008986
			0.010000	102	0.007058	0.001864	102	0.004787	0.001864
			0.001000	684	0.000811	0.000000	4216	0.000967	0.000000
			0.000100	67379	0.000019	0.000000	—	—	—
			0.000010	258573	0.000002	0.000000	—	—	—
			0.000001	630765	0.000001	0.000000	—	—	—
sko56	77695	XGB E scp42	0.100000	102	0.011810	0.001864	3	0.097353	0.008986
			0.010000	159	0.003473	0.001529	102	0.004787	0.001864
			0.001000	684	0.000591	0.000000	4216	0.000967	0.000000
			0.000100	67379	0.000015	0.000000	—	—	—
			0.000010	258573	0.000002	0.000000	—	—	—
			0.000001	630765	0.000000	0.000000	—	—	—
sko56	78300	DTR C scp42	0.100000	2	0.064610	0.151038	14	0.056093	0.039668
			0.010000	1389	0.000636	0.000000	74	0.005512	0.001533
			0.001000	1389	0.000636	0.000000	15743	0.000836	0.000000
			0.000100	11923	0.000085	0.000000	—	—	—
			0.000010	136667	0.000005	0.000000	—	—	—
			0.000001	496220	0.000001	0.000000	—	—	—
sko56	78300	XGB E scp42	0.100000	14	0.016695	0.039668	14	0.056093	0.039668
			0.010000	1389	0.000638	0.000000	74	0.005512	0.001533
			0.001000	1389	0.000638	0.000000	15743	0.000836	0.000000
			0.000100	11923	0.000015	0.000000	—	—	—
			0.000010	136667	0.000004	0.000000	—	—	—
			0.000001	496220	0.000001	0.000000	—	—	—
sko56	83970	DTR C scp42	0.100000	2	0.082691	0.482629	4	0.068746	0.040303
			0.010000	1848	0.000476	0.000000	228	0.002107	0.000029
			0.001000	1848	0.000476	0.000000	41688	0.000957	0.000000
			0.000100	11096	0.000085	0.000000	—	—	—
			0.000010	91099	0.000007	0.000000	—	—	—
			0.000001	757056	0.000000	0.000000	—	—	—
sko56	83970	XGB E scp42	0.100000	4	0.092657	0.040303	4	0.068746	0.040303
			0.010000	166	0.003479	0.005291	228	0.002107	0.000029
			0.001000	1848	0.000367	0.000000	41688	0.000957	0.000000
			0.000100	11096	0.000051	0.000000	—	—	—
			0.000010	91099	0.000006	0.000000	—	—	—
			0.000001	168303	0.000001	0.000000	—	—	—
tai30a	11224	DTR C scp42	0.100000	9	0.032036	0.101636	18	0.071930	0.085295
			0.010000	18	0.000615	0.085295	113	0.006880	0.029997

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	18	0.000615	0.085295	417	0.000439	0.000272
			0.000100	720039	0.000000	0.000000	1116	0.000002	0.000000
			0.000010	720039	0.000000	0.000000	1116	0.000002	0.000000
			0.000001	720039	0.000000	0.000000	—	—	—
tai30a	11224	XGB E scp42	0.100000	6	0.040127	0.192734	18	0.071930	0.085295
			0.010000	18	0.002063	0.085295	113	0.006880	0.029997
			0.001000	1116	0.000147	0.000000	417	0.000439	0.000272
			0.000100	720039	0.000000	0.000000	1116	0.000002	0.000000
			0.000010	720039	0.000000	0.000000	1116	0.000002	0.000000
			0.000001	720039	0.000000	0.000000	—	—	—
tai30a	17805	DTR C scp42	0.100000	10	0.032036	0.103940	10	0.012174	0.103940
			0.010000	119	0.007550	0.009038	119	0.006570	0.009038
			0.001000	752	0.000811	0.002082	3013	0.000673	0.000000
			0.000100	11859	0.000083	0.000000	18668	0.000002	0.000000
			0.000010	—	—	—	18668	0.000002	0.000000
			0.000001	—	—	—	—	—	—
tai30a	17805	XGB E scp42	0.100000	10	0.011121	0.103940	10	0.012174	0.103940
			0.010000	36	0.007142	0.026252	119	0.006570	0.009038
			0.001000	752	0.000982	0.002082	3013	0.000673	0.000000
			0.000100	11859	0.000052	0.000000	18668	0.000002	0.000000
			0.000010	—	—	—	18668	0.000002	0.000000
			0.000001	—	—	—	—	—	—
tai30a	19406	DTR C scp42	0.100000	19	0.000615	0.154630	20	0.090179	0.102034
			0.010000	19	0.000615	0.154630	70	0.008045	0.007889
			0.001000	19	0.000615	0.154630	495	0.000074	0.000000
			0.000100	35637	0.000028	0.000000	495	0.000074	0.000000
			0.000010	109878	0.000006	0.000000	109878	0.000002	0.000000
			0.000001	884237	0.000000	0.000000	884237	0.000001	0.000000
tai30a	19406	XGB E scp42	0.100000	14	0.034743	0.159518	20	0.090179	0.102034
			0.010000	19	0.002383	0.154630	70	0.008045	0.007889
			0.001000	35637	0.000033	0.000000	495	0.000074	0.000000
			0.000100	35637	0.000033	0.000000	495	0.000074	0.000000
			0.000010	109878	0.000006	0.000000	109878	0.000002	0.000000
			0.000001	884237	0.000000	0.000000	884237	0.000001	0.000000
tai30a	20374	DTR C scp42	0.100000	20	0.000615	0.055740	6	0.054723	0.058967
			0.010000	20	0.000615	0.055740	91	0.005320	0.003592
			0.001000	20	0.000615	0.055740	253	0.000793	0.000373
			0.000100	13742	0.000069	0.000000	14645	0.000017	0.000000
			0.000010	906583	0.000000	0.000000	64178	0.000006	0.000000
			0.000001	906583	0.000000	0.000000	—	—	—
tai30a	20374	XGB E scp42	0.100000	6	0.080043	0.058967	6	0.054723	0.058967
			0.010000	91	0.008050	0.003592	91	0.005320	0.003592
			0.001000	13742	0.000051	0.000000	253	0.000793	0.000373
			0.000100	13742	0.000051	0.000000	14645	0.000017	0.000000
			0.000010	906583	0.000000	0.000000	64178	0.000006	0.000000
			0.000001	906583	0.000000	0.000000	—	—	—
tai30a	25111	DTR C scp42	0.100000	64	0.009944	0.040007	64	0.030405	0.040007
			0.010000	64	0.009944	0.040007	72	0.006337	0.005056
			0.001000	990	0.000682	0.000656	3451	0.000438	0.000000
			0.000100	24740	0.000028	0.000000	35895	0.000040	0.000000
			0.000010	157006	0.000005	0.000000	332402	0.000009	0.000000
			0.000001	434887	0.000001	0.000000	—	—	—
tai30a	25111	XGB E scp42	0.100000	6	0.080365	0.086862	64	0.030405	0.040007
			0.010000	293	0.003272	0.004626	72	0.006337	0.005056
			0.001000	990	0.000471	0.000656	3451	0.000438	0.000000
			0.000100	24740	0.000027	0.000000	35895	0.000040	0.000000
			0.000010	157006	0.000004	0.000000	332402	0.000009	0.000000

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	434887	0.000001	0.000000	—	—	—
tai30a	47321	DTR C scp42	0.100000	22	0.016782	0.000728	3	0.084233	0.007176
			0.010000	1074	0.000682	0.000000	22	0.007281	0.000728
			0.001000	1074	0.000682	0.000000	1074	0.000574	0.000000
			0.000100	12016	0.000083	0.000000	19170	0.000060	0.000000
			0.000010	134568	0.000005	0.000000	134568	0.000002	0.000000
			0.000001	—	—	—	269843	0.000000	0.000000
tai30a	47321	XGB E scp42	0.100000	22	0.000537	0.000728	3	0.084233	0.007176
			0.010000	22	0.000537	0.000728	22	0.007281	0.000728
			0.001000	22	0.000537	0.000728	1074	0.000574	0.000000
			0.000100	7293	0.000022	0.000000	19170	0.000060	0.000000
			0.000010	134568	0.000004	0.000000	134568	0.000002	0.000000
			0.000001	—	—	—	269843	0.000000	0.000000
tai30a	79669	DTR C scp42	0.100000	16	0.000615	0.054757	7	0.062955	0.068620
			0.010000	16	0.000615	0.054757	58	0.000226	0.000010
			0.001000	16	0.000615	0.054757	58	0.000226	0.000010
			0.000100	253642	0.000002	0.000000	2288	0.000039	0.000000
			0.000010	253642	0.000002	0.000000	6490	0.000005	0.000000
			0.000001	554128	0.000001	0.000000	793632	0.000001	0.000000
tai30a	79669	XGB E scp42	0.100000	7	0.091220	0.068620	7	0.062955	0.068620
			0.010000	42	0.006959	0.029953	58	0.000226	0.000010
			0.001000	2288	0.000480	0.000000	58	0.000226	0.000010
			0.000100	6490	0.000014	0.000000	2288	0.000039	0.000000
			0.000010	253642	0.000002	0.000000	6490	0.000005	0.000000
			0.000001	554128	0.000001	0.000000	793632	0.000001	0.000000
tai30a	82866	DTR C scp42	0.100000	9	0.032036	0.044192	9	0.043703	0.044192
			0.010000	17	0.000615	0.042919	149	0.009125	0.010101
			0.001000	17	0.000615	0.042919	962	0.000826	0.000000
			0.000100	33417	0.000028	0.000000	5984	0.000093	0.000000
			0.000010	108626	0.000006	0.000000	46187	0.000009	0.000000
			0.000001	—	—	—	—	—	—
tai30a	82866	XGB E scp42	0.100000	9	0.052438	0.044192	9	0.043703	0.044192
			0.010000	231	0.006434	0.002182	149	0.009125	0.010101
			0.001000	1236	0.000151	0.000000	962	0.000826	0.000000
			0.000100	5984	0.000098	0.000000	5984	0.000093	0.000000
			0.000010	108626	0.000002	0.000000	46187	0.000009	0.000000
			0.000001	257742	0.000001	0.000000	—	—	—
tai30a	93222	DTR C scp42	0.100000	21	0.041670	0.023366	5	0.030314	0.061897
			0.010000	216	0.001465	0.009967	46	0.008983	0.012453
			0.001000	683	0.000811	0.003640	803	0.000988	0.000406
			0.000100	10440	0.000083	0.000000	13243	0.000061	0.000000
			0.000010	129167	0.000006	0.000000	204299	0.000002	0.000000
			0.000001	—	—	—	257467	0.000001	0.000000
tai30a	93222	XGB E scp42	0.100000	21	0.011795	0.023366	5	0.030314	0.061897
			0.010000	216	0.001132	0.009967	46	0.008983	0.012453
			0.001000	262	0.000710	0.005086	803	0.000988	0.000406
			0.000100	10440	0.000083	0.000000	13243	0.000061	0.000000
			0.000010	129167	0.000002	0.000000	204299	0.000002	0.000000
			0.000001	133817	0.000001	0.000000	257467	0.000001	0.000000
tai30a	95593	DTR C scp42	0.100000	11	0.032036	0.020606	5	0.090725	0.035537
			0.010000	107	0.007307	0.000056	107	0.001073	0.000056
			0.001000	11805	0.000083	0.000000	536	0.000087	0.000000
			0.000100	11805	0.000083	0.000000	536	0.000087	0.000000
			0.000010	217231	0.000002	0.000000	217231	0.000004	0.000000
			0.000001	497252	0.000001	0.000000	672516	0.000001	0.000000
tai30a	95593	XGB E scp42	0.100000	5	0.034232	0.035537	5	0.090725	0.035537
			0.010000	49	0.008300	0.004000	107	0.001073	0.000056

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.001000	11805	0.000059	0.000000	536	0.000087	0.000000
			0.000100	11805	0.000059	0.000000	536	0.000087	0.000000
			0.000010	83333	0.000008	0.000000	217231	0.000004	0.000000
			0.000001	497252	0.000001	0.000000	672516	0.000001	0.000000
wil50	17865	DTR C scp42	0.100000	2	0.038658	0.775968	4	0.045220	0.226096
			0.010000	6	0.000722	0.184698	171	0.008049	0.000375
			0.001000	6	0.000722	0.184698	889615	0.000867	0.000000
			0.000100	28707	0.000028	0.000000	—	—	—
			0.000010	294806	0.000002	0.000000	—	—	—
			0.000001	889615	0.000000	0.000000	—	—	—
wil50	17865	XGB E scp42	0.100000	4	0.092657	0.226096	4	0.045220	0.226096
			0.010000	37	0.007898	0.025646	171	0.008049	0.000375
			0.001000	1145	0.000507	0.000000	889615	0.000867	0.000000
			0.000100	28707	0.000030	0.000000	—	—	—
			0.000010	294806	0.000002	0.000000	—	—	—
			0.000001	889615	0.000000	0.000000	—	—	—
wil50	23781	DTR C scp42	0.100000	2	0.038658	0.557025	7	0.061020	0.268233
			0.010000	7	0.000722	0.268233	9	0.009779	0.008044
			0.001000	7	0.000722	0.268233	—	—	—
			0.000100	27077	0.000028	0.000000	—	—	—
			0.000010	129244	0.000006	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	23781	XGB E scp42	0.100000	7	0.070790	0.268233	7	0.061020	0.268233
			0.010000	377	0.000927	0.001584	9	0.009779	0.008044
			0.001000	377	0.000927	0.001584	—	—	—
			0.000100	6555	0.000015	0.000000	—	—	—
			0.000010	129244	0.000004	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	24962	DTR C scp42	0.100000	2	0.038658	0.432945	6	0.020268	0.045045
			0.010000	6	0.000722	0.045045	71	0.004402	0.000653
			0.001000	6	0.000722	0.045045	164416	0.000242	0.000000
			0.000100	12036	0.000085	0.000000	—	—	—
			0.000010	164416	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	24962	XGB E scp42	0.100000	6	0.076935	0.045045	6	0.020268	0.045045
			0.010000	29	0.009992	0.020497	71	0.004402	0.000653
			0.001000	398	0.000801	0.000000	164416	0.000242	0.000000
			0.000100	12036	0.000037	0.000000	—	—	—
			0.000010	164416	0.000003	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	47019	DTR C scp42	0.100000	2	0.038658	0.390185	5	0.091368	0.288938
			0.010000	5	0.000722	0.288938	213	0.004053	0.000710
			0.001000	5	0.000722	0.288938	721572	0.000686	0.000000
			0.000100	63766	0.000019	0.000000	—	—	—
			0.000010	157972	0.000005	0.000000	—	—	—
			0.000001	721572	0.000000	0.000000	—	—	—
wil50	47019	XGB E scp42	0.100000	5	0.073736	0.288938	5	0.091368	0.288938
			0.010000	14	-0.003185	0.163454	213	0.004053	0.000710
			0.001000	14	-0.003185	0.163454	721572	0.000686	0.000000
			0.000100	14	-0.003185	0.163454	—	—	—
			0.000010	14	-0.003185	0.163454	—	—	—
			0.000001	14	-0.003185	0.163454	—	—	—
wil50	49622	DTR C scp42	0.100000	2	0.038658	0.645251	4	0.044768	0.219846
			0.010000	12	0.000722	0.015149	200	0.008939	0.000605
			0.001000	12	0.000722	0.015149	682619	0.000880	0.000000
			0.000100	10425	0.000078	0.000000	—	—	—
			0.000010	131903	0.000005	0.000000	—	—	—

Instance	Seed	Model	β	Iteration (ML S.)	Probs. (ML S.)	Expected (ML S.)	Iteration (Prob. S.)	Probs. (Prob. S.)	Expected (Prob. S.)
			0.000001	682619	0.000000	0.000000	—	—	—
wil50	49622	XGB E scp42	0.100000	4	0.092714	0.219846	4	0.044768	0.219846
			0.010000	165	0.002940	0.005695	200	0.008939	0.000605
			0.001000	209	0.000941	0.000035	682619	0.000880	0.000000
			0.000100	7386	0.000037	0.000000	—	—	—
			0.000010	131903	0.000005	0.000000	—	—	—
			0.000001	682619	0.000000	0.000000	—	—	—
wil50	52215	DTR C scp42	0.100000	2	0.038658	0.400277	8	0.048945	0.014454
			0.010000	5	0.000722	0.180681	1208	0.007372	0.000000
			0.001000	5	0.000722	0.180681	490180	0.000878	0.000000
			0.000100	12448	0.000085	0.000000	—	—	—
			0.000010	100456	0.000007	0.000000	—	—	—
			0.000001	490180	0.000001	0.000000	—	—	—
wil50	52215	XGB E scp42	0.100000	5	0.071295	0.180681	8	0.048945	0.014454
			0.010000	267	0.000701	0.000392	1208	0.007372	0.000000
			0.001000	267	0.000701	0.000392	490180	0.000878	0.000000
			0.000100	12448	0.000052	0.000000	—	—	—
			0.000010	69912	0.000009	0.000000	—	—	—
			0.000001	203748	0.000001	0.000000	—	—	—
wil50	75302	DTR C scp42	0.100000	2	0.038658	0.543690	4	0.071377	0.174011
			0.010000	6	0.000722	0.031953	430	0.004050	0.000000
			0.001000	6	0.000722	0.031953	83959	0.000943	0.000000
			0.000100	28653	0.000028	0.000000	—	—	—
			0.000010	538921	0.000001	0.000000	—	—	—
			0.000001	538921	0.000001	0.000000	—	—	—
wil50	75302	XGB E scp42	0.100000	6	0.076935	0.031953	4	0.071377	0.174011
			0.010000	130	0.005282	0.003203	430	0.004050	0.000000
			0.001000	430	0.000668	0.000000	83959	0.000943	0.000000
			0.000100	28653	0.000040	0.000000	—	—	—
			0.000010	538921	0.000001	0.000000	—	—	—
			0.000001	538921	0.000001	0.000000	—	—	—
wil50	75860	DTR C scp42	0.100000	2	0.038658	0.588125	3	0.086278	0.309105
			0.010000	15	0.000615	0.024359	539	0.006988	0.000383
			0.001000	15	0.000615	0.024359	—	—	—
			0.000100	15665	0.000069	0.000000	—	—	—
			0.000010	122145	0.000006	0.000000	—	—	—
			0.000001	370206	0.000001	0.000000	—	—	—
wil50	75860	XGB E scp42	0.100000	15	0.007322	0.024359	3	0.086278	0.309105
			0.010000	15	0.007322	0.024359	539	0.006988	0.000383
			0.001000	3130	0.000386	0.000000	—	—	—
			0.000100	15665	0.000074	0.000000	—	—	—
			0.000010	122145	0.000005	0.000000	—	—	—
			0.000001	370206	0.000001	0.000000	—	—	—
wil50	84494	DTR C scp42	0.100000	2	0.038658	0.603006	3	0.078179	0.059452
			0.010000	33	0.000136	0.000811	1786	0.005194	0.000000
			0.001000	33	0.000136	0.000811	149064	0.000635	0.000000
			0.000100	16448	0.000069	0.000000	—	—	—
			0.000010	149064	0.000005	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	84494	XGB E scp42	0.100000	31	0.017824	0.041889	3	0.078179	0.059452
			0.010000	1786	0.000553	0.000000	1786	0.005194	0.000000
			0.001000	1786	0.000553	0.000000	149064	0.000635	0.000000
			0.000100	9013	0.000049	0.000000	—	—	—
			0.000010	149064	0.000003	0.000000	—	—	—
			0.000001	—	—	—	—	—	—
wil50	88252	DTR C scp42	0.100000	2	0.038658	0.078149	27	0.035615	0.022955
			0.010000	5	0.000722	0.063358	790	0.007491	0.000000

Instance	Seed	Model	β	**Iteration (ML S.)**	**Probs. (ML S.)**	**Expected (ML S.)**	**Iteration (Prob. S.)**	**Probs. (Prob. S.)**	**Expected (Prob. S.)**
			0.001000	5	0.000722	0.063358	409738	0.000565	0.000000
			0.000100	41	0.000041	0.006120	—	—	—
			0.000010	340792	0.000002	0.000000	—	—	—
			0.000001	409738	0.000001	0.000000	—	—	—
wil50	88252	XGB E scp42	0.100000	5	0.067689	0.063358	27	0.035615	0.022955
			0.010000	27	0.009992	0.022955	790	0.007491	0.000000
			0.001000	790	0.000467	0.000000	409738	0.000565	0.000000
			0.000100	38284	0.000029	0.000000	—	—	—
			0.000010	340792	0.000002	0.000000	—	—	—
			0.000001	409738	0.000001	0.000000	—	—	—